



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 02:52 am GMT

PDB ID : 4UQV  
Title : methanococcus jannaschii serine hydroxymethyl-transferase in complex with PLP  
Authors : Saccoccia, F.; Angelucci, F.; Ilari, A.  
Deposited on : 2014-06-25  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

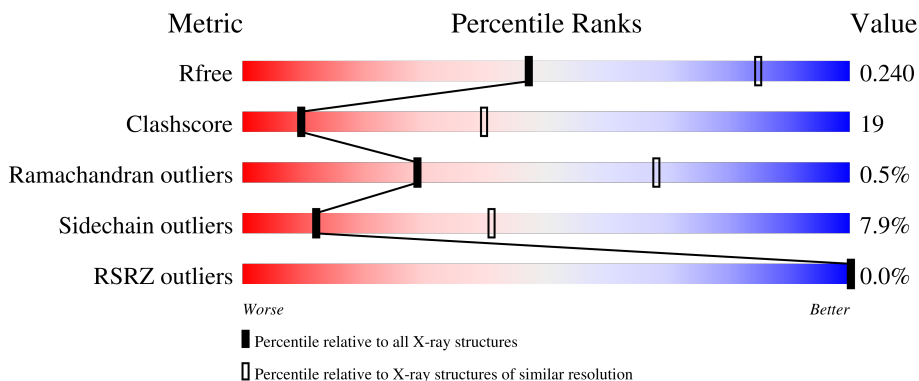
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



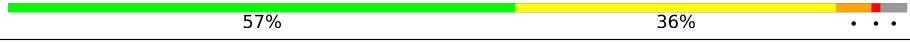






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	61% (green), 34% (yellow), 5% (orange), 0% (red), 0% (grey)
1	B	429	60% (green), 36% (yellow), 4% (orange), 0% (red), 0% (grey)
1	C	429	59% (green), 36% (yellow), 5% (orange), 0% (red), 0% (grey)
1	D	429	57% (green), 36% (yellow), 6% (orange), 0% (red), 0% (grey)
1	E	429	52% (green), 43% (yellow), 5% (orange), 0% (red), 0% (grey)

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Mol	Chain	Length	Quality of chain
1	F	429	 57% 36% . . .
1	G	429	 57% 38% 5%
1	H	429	 57% 39% .
1	I	429	 59% 36% .
1	J	429	 54% 43% .
1	K	429	 57% 37% . .
1	L	429	 56% 36% 6% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	Total 3362	C 2146	N 560	O 639	S 17	0	0	0
1	B	424	Total 3344	C 2133	N 558	O 636	S 17	0	0	0
1	C	420	Total 3308	C 2112	N 552	O 628	S 16	0	0	0
1	D	425	Total 3354	C 2141	N 559	O 638	S 16	0	0	0
1	E	427	Total 3369	C 2150	N 565	O 638	S 16	0	0	0
1	F	418	Total 3300	C 2107	N 554	O 623	S 16	0	0	0
1	G	429	Total 3386	C 2160	N 567	O 642	S 17	0	0	0
1	H	427	Total 3366	C 2146	N 564	O 639	S 17	0	0	0
1	I	427	Total 3369	C 2150	N 565	O 638	S 16	0	0	0
1	J	429	Total 3386	C 2160	N 567	O 642	S 17	0	0	0
1	K	422	Total 3329	C 2125	N 559	O 629	S 16	0	0	0
1	L	420	Total 3317	C 2122	N 555	O 624	S 16	0	0	0

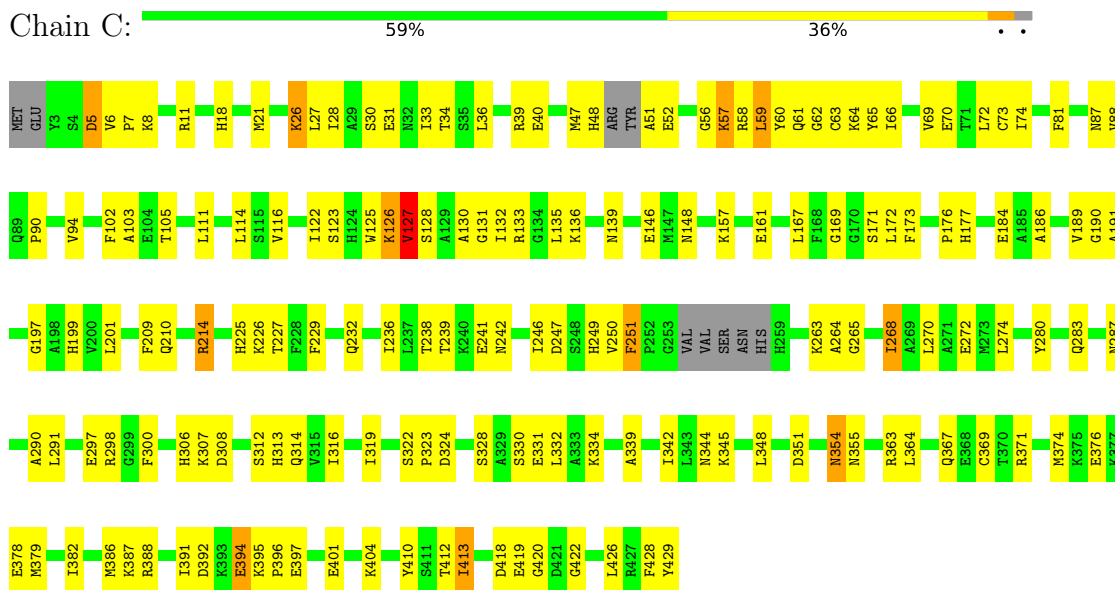
- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



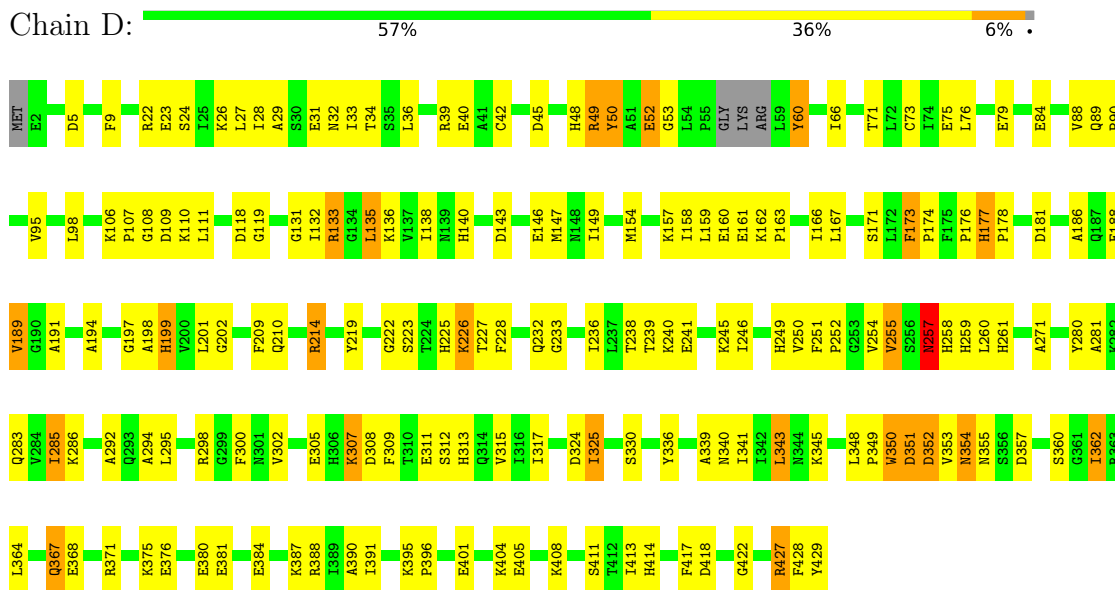
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 15	8	1	5	1	0	0
2	B	1	Total 15	8	1	5	1	0	0
2	C	1	Total 15	8	1	5	1	0	0
2	D	1	Total 15	8	1	5	1	0	0
2	E	1	Total 15	8	1	5	1	0	0
2	F	1	Total 15	8	1	5	1	0	0
2	G	1	Total 15	8	1	5	1	0	0
2	H	1	Total 15	8	1	5	1	0	0
2	I	1	Total 15	8	1	5	1	0	0
2	J	1	Total 15	8	1	5	1	0	0
2	K	1	Total 15	8	1	5	1	0	0
2	L	1	Total 15	8	1	5	1	0	0



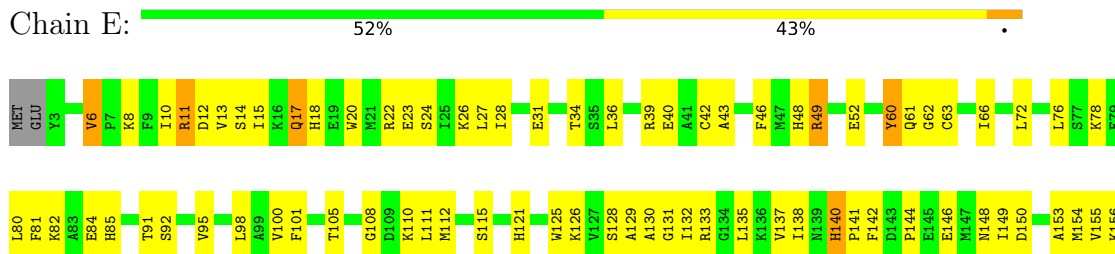
● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

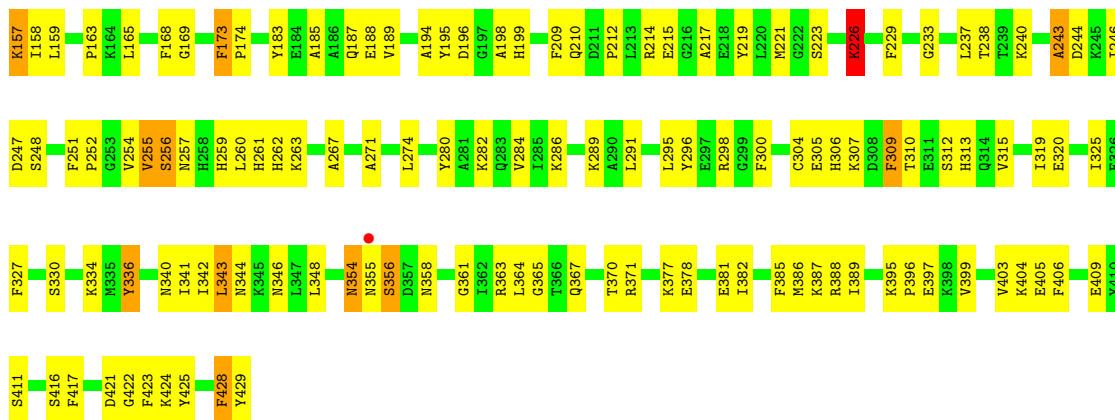


● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



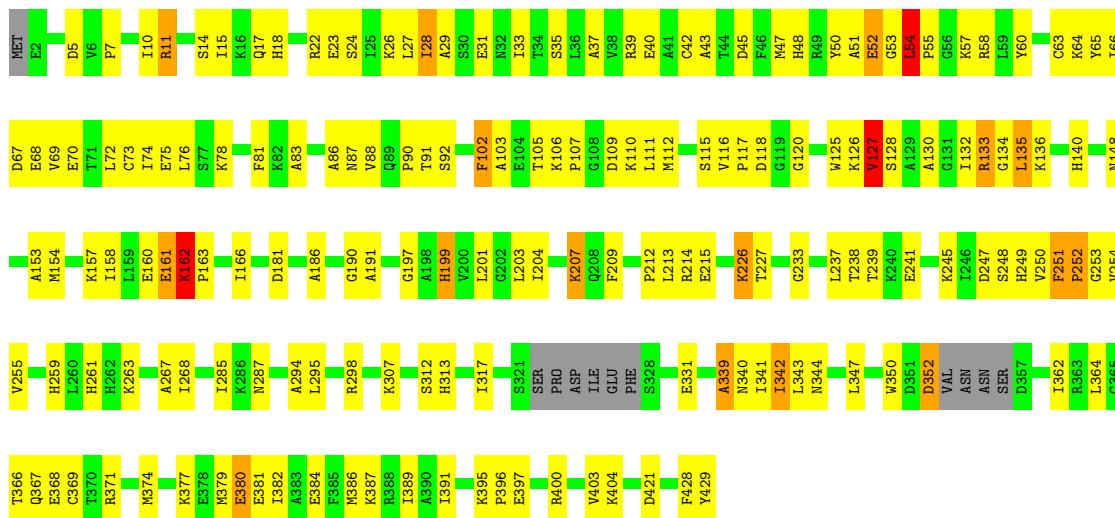
● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE





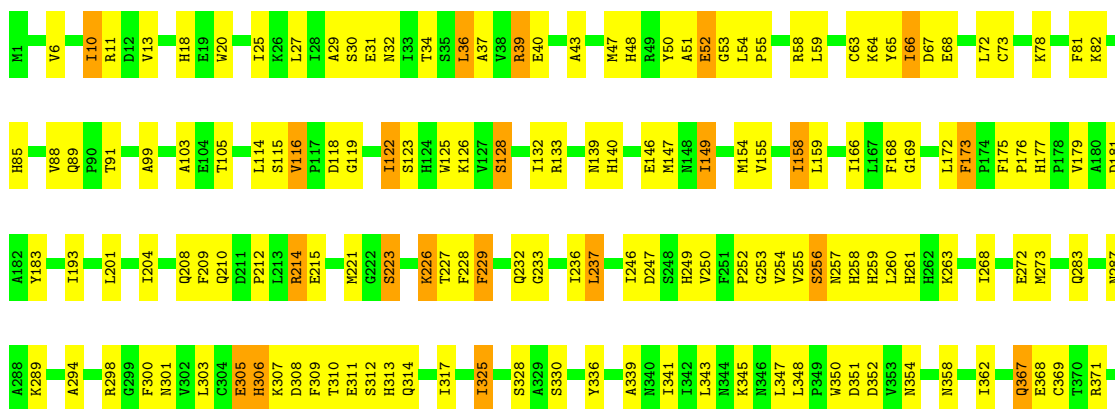
● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain F: 57% 36%



● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

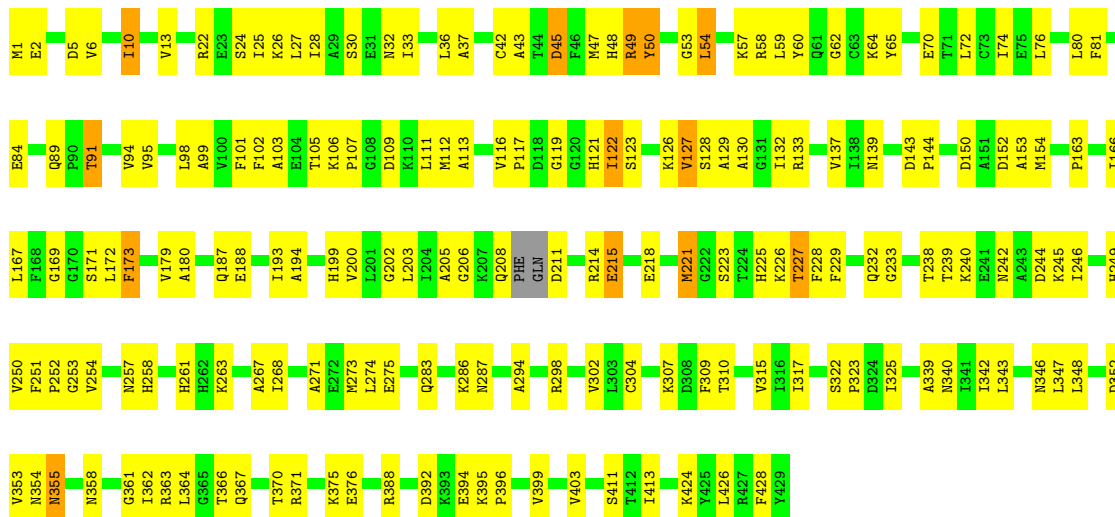
Chain G: 57% 38% 5%



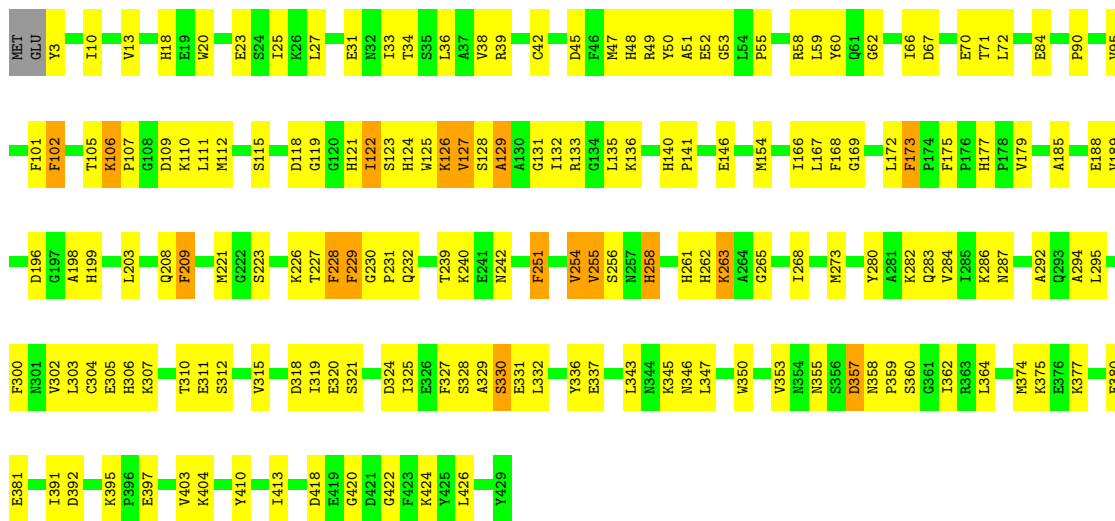




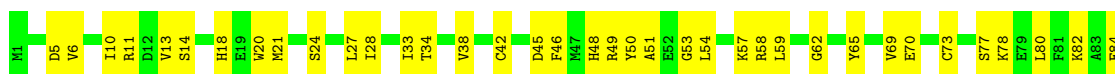
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.13Å 47.16Å 344.08Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.15 – 3.00 49.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-3.00) 90.7 (49.15-3.00)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1702)	Depositor
R, $R_{free}$	0.198 , 0.243 0.202 , 0.240	Depositor DCC
$R_{free}$ test set	4050 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 80986 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	40370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/3437	0.48	0/4635
1	B	0.28	1/3417 (0.0%)	0.54	6/4606 (0.1%)
1	C	0.26	0/3380	0.49	1/4554 (0.0%)
1	D	0.26	0/3429	0.52	0/4625
1	E	0.25	0/3445	0.55	3/4646 (0.1%)
1	F	0.26	0/3372	0.53	2/4542 (0.0%)
1	G	0.26	0/3462	0.47	0/4668
1	H	0.25	0/3440	0.50	1/4637 (0.0%)
1	I	0.25	0/3445	0.52	3/4646 (0.1%)
1	J	0.27	0/3462	0.55	3/4668 (0.1%)
1	K	0.25	0/3402	0.50	1/4584 (0.0%)
1	L	0.24	0/3389	0.47	0/4563
All	All	0.26	1/41080 (0.0%)	0.51	20/55374 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	5
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	1
1	I	0	3
1	J	0	1
1	K	0	3
1	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	PRO	N-CD	5.21	1.55	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	226	LYS	N-CA-C	9.70	137.19	111.00
1	E	226	LYS	N-CA-C	9.53	136.72	111.00
1	B	226	LYS	N-CA-C	9.24	135.94	111.00
1	I	226	LYS	N-CA-C	8.29	133.38	111.00
1	J	254	VAL	CB-CA-C	-7.69	96.79	111.40
1	B	255	VAL	CB-CA-C	7.46	125.57	111.40
1	H	54	LEU	CB-CA-C	7.20	123.87	110.20
1	F	54	LEU	CB-CA-C	7.08	123.65	110.20
1	J	226	LYS	CB-CA-C	-6.91	96.57	110.40
1	I	226	LYS	CB-CA-C	-6.83	96.75	110.40
1	F	251	PHE	C-N-CD	6.60	142.25	128.40
1	B	226	LYS	CB-CA-C	-6.30	97.79	110.40
1	E	226	LYS	CB-CA-C	-6.21	97.97	110.40
1	B	255	VAL	N-CA-C	-5.34	96.58	111.00
1	K	392	ASP	CB-CA-C	-5.34	99.72	110.40
1	I	129	ALA	CB-CA-C	-5.28	102.17	110.10
1	B	251	PHE	C-N-CD	5.28	139.49	128.40
1	C	226	LYS	N-CA-C	5.27	125.22	111.00
1	E	309	PHE	CB-CA-C	-5.23	99.94	110.40
1	B	257	ASN	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	VAL	Peptide
1	A	255	VAL	Peptide
1	A	256	SER	Peptide
1	B	226	LYS	Peptide
1	B	256	SER	Peptide
1	C	251	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	C	308	ASP	Peptide
1	C	354	ASN	Peptide
1	C	355	ASN	Peptide
1	C	56	GLY	Peptide
1	D	257	ASN	Peptide
1	D	350	TRP	Peptide
1	D	351	ASP	Peptide
1	E	226	LYS	Peptide
1	E	356	SER	Peptide
1	F	339	ALA	Peptide
1	F	52	GLU	Peptide
1	G	253	GLY	Peptide
1	I	126	LYS	Peptide
1	I	251	PHE	Peptide
1	I	254	VAL	Peptide
1	J	128	SER	Peptide
1	K	107	PRO	Peptide
1	K	109	ASP	Peptide
1	K	354	ASN	Peptide
1	L	250	VAL	Peptide
1	L	251	PHE	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3362	0	3304	132	0
1	B	3344	0	3288	149	0
1	C	3308	0	3257	134	0
1	D	3354	0	3292	177	0
1	E	3369	0	3316	157	0
1	F	3300	0	3252	138	0
1	G	3386	0	3334	152	0
1	H	3366	0	3316	132	0
1	I	3369	0	3316	147	0
1	J	3386	0	3335	137	0
1	K	3329	0	3281	134	0
1	L	3317	0	3269	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	7	2	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	0	0
2	E	15	0	7	2	0
2	F	15	0	7	2	0
2	G	15	0	7	1	0
2	H	15	0	7	0	0
2	I	15	0	7	0	0
2	J	15	0	7	1	0
2	K	15	0	7	0	0
2	L	15	0	7	0	0
All	All	40370	0	39644	1550	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1550) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:GLU:HG2	1:I:60:TYR:CD1	1.70	1.24
1:D:351:ASP:HB2	1:D:352:ASP:OD1	1.44	1.16
1:A:310:THR:HG23	1:A:311:GLU:N	1.55	1.12
1:C:47:MET:HE1	1:D:34:THR:HG21	1.25	1.11
1:A:147:MET:HB2	1:A:175:PHE:HE2	1.08	1.09
1:C:47:MET:CE	1:D:34:THR:HG21	1.83	1.08
1:A:310:THR:CG2	1:A:311:GLU:H	1.69	1.04
1:A:147:MET:HB2	1:A:175:PHE:CE2	1.97	0.99
1:A:310:THR:HG23	1:A:311:GLU:H	0.82	0.98
1:D:351:ASP:CB	1:D:352:ASP:OD1	2.12	0.97
1:I:52:GLU:CG	1:I:60:TYR:CD1	2.47	0.96
1:A:310:THR:CG2	1:A:311:GLU:N	2.25	0.96
1:B:251:PHE:HB3	1:B:252:PRO:HD3	1.51	0.91
1:A:310:THR:CG2	1:A:312:SER:H	1.84	0.89
1:C:48:HIS:NE2	1:D:34:THR:HG22	1.88	0.89
1:D:353:VAL:O	1:D:354:ASN:ND2	2.07	0.88
1:I:52:GLU:CD	1:I:60:TYR:HD1	1.77	0.88
1:A:310:THR:HG23	1:A:312:SER:H	1.36	0.88
1:K:59:LEU:HB3	1:L:345:LYS:HE2	1.56	0.87
1:A:50:TYR:CD2	1:B:30:SER:HB3	2.09	0.86
1:K:135:LEU:HB3	1:K:136:LYS:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:LYS:HB3	1:E:310:THR:HG22	1.59	0.84
1:I:52:GLU:CG	1:I:60:TYR:HD1	1.90	0.84
1:I:127:VAL:HG13	1:I:128:SER:H	1.43	0.82
1:B:251:PHE:O	1:B:255:VAL:HG12	1.78	0.82
1:L:198:ALA:HA	1:L:223:SER:H	1.44	0.81
1:E:289:LYS:HB3	1:E:310:THR:CG2	2.10	0.81
1:H:353:VAL:HG12	1:H:355:ASN:H	1.46	0.79
1:K:251:PHE:N	1:K:253:GLY:H	1.81	0.78
1:B:250:VAL:O	1:B:255:VAL:HB	1.83	0.78
1:B:251:PHE:HB3	1:B:252:PRO:CD	2.13	0.78
1:K:7:PRO:HA	1:K:10:ILE:HD12	1.65	0.78
1:A:147:MET:CB	1:A:175:PHE:HE2	1.94	0.78
1:E:10:ILE:HD12	1:F:268:ILE:HG13	1.64	0.78
1:C:40:GLU:HG3	1:D:428:PHE:HD1	1.49	0.77
1:J:287:ASN:HB3	1:J:366:THR:HG21	1.65	0.77
1:D:202:GLY:HA3	1:D:227:THR:O	1.85	0.77
1:D:33:ILE:HB	1:D:368:GLU:HG3	1.67	0.77
1:D:251:PHE:H	1:D:254:VAL:HG12	1.50	0.77
1:G:388:ARG:HA	1:G:392:ASP:HB2	1.65	0.76
1:C:127:VAL:O	1:D:252:PRO:HB2	1.84	0.76
1:I:101:PHE:HD2	1:I:129:ALA:O	1.68	0.76
1:L:38:VAL:HG11	1:L:230:GLY:HA2	1.67	0.76
1:A:133:ARG:HB2	1:B:132:ILE:HG23	1.67	0.75
1:I:324:ASP:HB3	1:I:391:ILE:HG23	1.68	0.75
1:A:198:ALA:HA	1:A:223:SER:H	1.52	0.75
1:F:160:GLU:O	1:F:161:GLU:HG3	1.87	0.74
1:A:203:LEU:HG	1:A:227:THR:HG21	1.69	0.74
1:B:251:PHE:HA	1:B:255:VAL:HG11	1.70	0.74
1:D:199:HIS:HA	1:D:226:LYS:HD2	1.68	0.74
1:D:325:ILE:HB	1:D:391:ILE:HA	1.70	0.74
1:B:248:SER:HA	1:B:252:PRO:HD2	1.71	0.73
1:E:23:GLU:HB2	1:E:404:LYS:HG3	1.71	0.73
1:I:51:ALA:O	1:I:52:GLU:HG3	1.87	0.73
1:L:49:ARG:NH2	1:L:62:GLY:O	2.22	0.73
1:B:53:GLY:H	1:B:251:PHE:HE2	1.34	0.73
1:B:87:ASN:ND2	1:B:250:VAL:HG21	2.04	0.73
1:D:23:GLU:HG2	1:D:408:LYS:HD3	1.71	0.73
1:E:255:VAL:HG12	1:E:256:SER:N	2.04	0.72
1:K:100:VAL:HG11	1:K:221:MET:HG2	1.70	0.72
1:G:36:LEU:HD11	1:G:420:GLY:HA3	1.72	0.71
1:B:87:ASN:HD21	1:B:250:VAL:HG21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ARG:NH1	1:D:414:HIS:O	2.23	0.71
1:H:50:TYR:CE1	1:H:257:ASN:HB3	2.26	0.71
1:K:39:ARG:NH1	1:K:422:GLY:O	2.23	0.71
1:E:130:ALA:O	1:E:135:LEU:N	2.23	0.70
1:A:199:HIS:HA	1:A:226:LYS:HG2	1.72	0.70
1:J:146:GLU:HG3	1:J:307:LYS:HD2	1.73	0.70
1:I:319:ILE:HD13	1:I:332:LEU:HD23	1.74	0.70
1:B:348:LEU:H	1:B:351:ASP:HB2	1.54	0.70
1:F:11:ARG:NH2	1:F:429:TYR:O	2.25	0.70
1:G:73:CYS:HB3	1:G:88:VAL:HG11	1.74	0.70
1:I:13:VAL:HG13	1:J:65:TYR:HB3	1.73	0.70
1:K:337:GLU:OE1	1:L:61:GLN:NE2	2.25	0.70
1:C:40:GLU:HG3	1:D:428:PHE:CD1	2.26	0.70
1:A:110:LYS:HB3	1:A:163:PRO:HA	1.73	0.69
1:F:33:ILE:H	1:F:368:GLU:HG3	1.55	0.69
1:K:51:ALA:O	1:K:58:ARG:NH1	2.25	0.69
1:E:92:SER:HB3	1:E:95:VAL:HG13	1.74	0.69
1:F:400:ARG:HE	1:F:404:LYS:HZ1	1.40	0.69
1:B:50:TYR:CE1	1:B:257:ASN:HB3	2.28	0.69
1:B:251:PHE:HD1	1:B:252:PRO:CD	2.05	0.69
1:E:428:PHE:HB2	1:F:40:GLU:HB2	1.74	0.69
1:I:251:PHE:CD2	1:I:251:PHE:O	2.46	0.69
1:G:133:ARG:NH1	1:H:132:ILE:O	2.26	0.68
1:I:101:PHE:CD2	1:I:129:ALA:O	2.46	0.68
1:C:388:ARG:HA	1:C:392:ASP:HB2	1.75	0.68
1:I:51:ALA:HB1	1:I:58:ARG:NH1	2.08	0.68
1:J:78:LYS:NZ	1:J:84:GLU:O	2.26	0.68
1:D:34:THR:HG23	1:D:39:ARG:HG3	1.74	0.68
1:F:27:LEU:HB3	1:F:364:LEU:HD22	1.76	0.68
1:A:256:SER:H	1:B:94:VAL:HG21	1.58	0.68
1:E:121:HIS:HB2	2:E:1430:PLP:H2A3	1.76	0.67
1:E:255:VAL:HG12	1:E:256:SER:H	1.58	0.67
1:C:26:LYS:HA	1:C:342:ILE:HB	1.74	0.67
1:L:39:ARG:NH2	1:L:422:GLY:O	2.28	0.67
1:I:258:HIS:O	1:I:263:LYS:NZ	2.28	0.67
1:B:256:SER:OG	1:B:257:ASN:N	2.27	0.67
1:C:229:PHE:HE1	1:C:272:GLU:HG3	1.59	0.67
1:E:251:PHE:O	1:E:251:PHE:CD2	2.48	0.67
1:I:231:PRO:HB2	1:I:262:HIS:HD2	1.60	0.67
1:K:325:ILE:HG22	1:K:327:PHE:H	1.60	0.67
1:F:110:LYS:HB3	1:F:163:PRO:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:THR:O	1:G:133:ARG:NH2	2.28	0.67
1:G:58:ARG:NH2	1:G:67:ASP:OD2	2.28	0.67
1:K:130:ALA:HA	1:K:134:GLY:H	1.60	0.67
1:E:111:LEU:HB3	1:E:137:VAL:HG12	1.77	0.66
1:E:31:GLU:O	1:E:367:GLN:NE2	2.28	0.66
1:A:298:ARG:NH1	1:A:384:GLU:OE1	2.29	0.66
1:E:330:SER:OG	1:E:334:LYS:NZ	2.28	0.66
1:A:225:HIS:NE2	2:A:1430:PLP:O3P	2.21	0.66
1:C:87:ASN:ND2	1:C:247:ASP:OD1	2.28	0.66
1:E:252:PRO:O	1:E:255:VAL:CG2	2.44	0.66
1:H:84:GLU:HB3	1:H:240:LYS:HG3	1.78	0.66
1:D:258:HIS:O	1:D:259:HIS:ND1	2.29	0.65
1:D:251:PHE:N	1:D:254:VAL:HG12	2.11	0.65
1:B:139:ASN:OD1	1:B:157:LYS:NZ	2.30	0.65
1:I:121:HIS:ND1	1:I:122:ILE:O	2.29	0.65
1:H:45:ASP:OD2	1:H:49:ARG:NE	2.29	0.65
1:H:123:SER:HB2	1:H:129:ALA:HB3	1.77	0.65
1:C:47:MET:CE	1:D:34:THR:CG2	2.70	0.65
1:L:261:HIS:HD1	1:L:261:HIS:H	1.43	0.65
1:B:251:PHE:HA	1:B:255:VAL:CG1	2.27	0.65
1:F:395:LYS:NZ	1:F:397:GLU:OE1	2.30	0.65
1:A:50:TYR:CE1	1:A:257:ASN:HB3	2.33	0.65
1:G:50:TYR:HD1	1:G:256:SER:HB2	1.61	0.65
1:A:325:ILE:HG12	1:A:390:ALA:HB1	1.79	0.64
1:B:246:ILE:O	1:B:250:VAL:HG12	1.96	0.64
1:E:14:SER:O	1:E:18:HIS:ND1	2.23	0.64
1:A:310:THR:HG23	1:A:312:SER:N	2.11	0.64
1:G:81:PHE:O	1:G:214:ARG:NH2	2.30	0.64
1:G:119:GLY:HA2	1:G:172:LEU:HD13	1.78	0.64
1:I:51:ALA:C	1:I:52:GLU:HG3	2.18	0.64
1:I:52:GLU:OE2	1:I:59:LEU:N	2.28	0.64
1:C:47:MET:HE2	1:D:34:THR:HG21	1.79	0.64
1:D:73:CYS:HB3	1:D:88:VAL:HG11	1.78	0.64
1:H:395:LYS:HD2	1:H:396:PRO:HD2	1.80	0.64
1:J:42:CYS:HA	1:J:261:HIS:HB2	1.80	0.64
1:B:247:ASP:HA	1:B:250:VAL:HG12	1.80	0.64
1:F:247:ASP:HA	1:F:250:VAL:HG12	1.78	0.64
1:I:345:LYS:NZ	1:I:357:ASP:O	2.31	0.64
1:A:319:ILE:HD11	1:A:362:ILE:HG13	1.80	0.64
1:G:212:PRO:HA	1:G:215:GLU:HB2	1.80	0.64
1:A:147:MET:CB	1:A:175:PHE:CE2	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:N	1:A:152:ASP:OD1	2.31	0.63
1:B:27:LEU:HG	1:B:364:LEU:HD23	1.80	0.63
1:B:353:VAL:HG23	1:B:355:ASN:H	1.62	0.63
1:H:200:VAL:HG13	1:H:203:LEU:HD12	1.81	0.63
1:I:310:THR:O	1:I:311:GLU:OE2	2.16	0.63
1:G:226:LYS:NZ	1:H:50:TYR:HE2	1.96	0.63
1:L:319:ILE:HD11	1:L:362:ILE:HB	1.80	0.63
1:D:283:GLN:HG2	1:D:375:LYS:HD2	1.79	0.63
1:G:255:VAL:HG22	1:H:94:VAL:HG11	1.79	0.63
1:D:300:PHE:HZ	1:D:390:ALA:HB3	1.62	0.63
1:E:28:ILE:HD13	1:F:60:TYR:HD2	1.64	0.63
1:I:52:GLU:CD	1:I:60:TYR:CD1	2.65	0.63
1:C:401:GLU:HA	1:C:404:LYS:HD2	1.81	0.63
1:K:17:GLN:OE1	1:L:49:ARG:NH1	2.31	0.63
1:E:10:ILE:HD11	1:F:267:ALA:HB3	1.81	0.63
1:E:49:ARG:NH2	1:E:62:GLY:O	2.28	0.62
1:L:84:GLU:HB3	1:L:240:LYS:HB3	1.81	0.62
1:B:254:VAL:O	1:B:254:VAL:HG22	1.99	0.62
1:D:295:LEU:HD13	1:D:317:ILE:HD11	1.80	0.62
1:F:35:SER:OG	1:F:371:ARG:NH2	2.33	0.62
1:J:405:GLU:HA	1:J:408:LYS:HB2	1.80	0.62
1:K:34:THR:O	1:K:39:ARG:NH2	2.32	0.62
1:E:411:SER:O	1:E:422:GLY:N	2.32	0.62
1:D:95:VAL:HG11	1:D:254:VAL:HG23	1.80	0.62
1:D:336:TYR:HB3	1:D:341:ILE:HB	1.80	0.62
1:F:58:ARG:NE	1:F:67:ASP:OD1	2.28	0.62
1:A:148:ASN:ND2	1:A:176:PRO:O	2.32	0.62
1:D:351:ASP:CA	1:D:352:ASP:OD1	2.47	0.62
1:J:162:LYS:HG2	1:J:189:VAL:HG22	1.80	0.62
1:D:29:ALA:HA	1:D:367:GLN:HE22	1.64	0.62
1:D:177:HIS:HB2	1:D:178:PRO:HD2	1.82	0.62
1:D:251:PHE:CD2	1:D:251:PHE:O	2.52	0.62
1:C:51:ALA:O	1:C:58:ARG:NH1	2.33	0.62
1:G:66:ILE:HG21	1:G:260:LEU:HD13	1.82	0.62
1:G:115:SER:HB3	1:G:118:ASP:HB2	1.82	0.62
1:K:38:VAL:HG11	1:K:269:ALA:HB2	1.82	0.62
1:B:251:PHE:CD1	1:B:252:PRO:HD3	2.34	0.61
1:F:340:ASN:HB2	1:F:403:VAL:CG2	2.29	0.61
1:I:282:LYS:HE3	1:I:286:LYS:HE2	1.81	0.61
1:B:325:ILE:HG23	1:B:326:GLU:H	1.64	0.61
1:F:14:SER:O	1:F:18:HIS:ND1	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:PHE:HB3	1:J:260:LEU:HB2	1.82	0.61
1:K:38:VAL:HG12	1:K:268:ILE:HB	1.82	0.61
1:B:27:LEU:O	1:B:365:GLY:N	2.33	0.61
1:C:6:VAL:HB	1:D:271:ALA:HB2	1.82	0.61
1:J:121:HIS:ND1	1:J:122:ILE:O	2.33	0.61
1:J:324:ASP:HB3	1:J:391:ILE:HD12	1.82	0.61
1:K:25:ILE:HG22	1:K:407:ALA:HB2	1.83	0.61
1:C:73:CYS:HB3	1:C:88:VAL:HG11	1.82	0.61
1:E:319:ILE:HG13	1:E:320:GLU:H	1.64	0.61
1:G:50:TYR:CD1	1:G:256:SER:HB2	2.35	0.61
1:C:270:LEU:O	1:C:274:LEU:HB2	2.01	0.61
1:H:187:GLN:HG2	1:K:137:VAL:HG12	1.83	0.61
1:G:306:HIS:HD2	1:G:307:LYS:HG3	1.65	0.60
1:J:254:VAL:O	1:J:254:VAL:HG12	2.01	0.60
1:D:313:HIS:HD2	1:D:367:GLN:HE21	1.48	0.60
1:F:340:ASN:HB2	1:F:403:VAL:HG23	1.82	0.60
1:B:73:CYS:HB3	1:B:88:VAL:HG11	1.84	0.60
1:F:91:THR:HG23	1:F:255:VAL:HG13	1.82	0.60
1:G:29:ALA:HA	1:G:367:GLN:HE22	1.66	0.60
1:C:291:LEU:HA	1:C:379:MET:HB3	1.83	0.60
1:E:209:PHE:HE1	1:E:312:SER:HB2	1.66	0.60
1:J:91:THR:O	1:J:94:VAL:HG22	2.01	0.60
1:D:353:VAL:HG22	1:D:355:ASN:H	1.66	0.60
1:G:229:PHE:CE1	1:G:272:GLU:HG3	2.36	0.60
1:K:367:GLN:N	1:K:367:GLN:OE1	2.32	0.60
1:L:272:GLU:OE2	1:L:371:ARG:NH2	2.34	0.60
1:A:271:ALA:HA	1:A:274:LEU:HB2	1.84	0.60
1:E:24:SER:O	1:E:26:LYS:NZ	2.35	0.60
1:G:339:ALA:HB2	1:G:396:PRO:HB3	1.82	0.60
1:H:89:GLN:HB2	1:H:250:VAL:HG11	1.82	0.60
1:L:250:VAL:HG23	1:L:254:VAL:H	1.67	0.60
1:D:24:SER:HA	1:D:340:ASN:HB3	1.83	0.60
1:G:132:ILE:HG22	1:H:133:ARG:HB2	1.83	0.60
1:L:255:VAL:O	1:L:258:HIS:N	2.34	0.60
1:C:39:ARG:NH1	1:C:422:GLY:O	2.35	0.60
1:I:33:ILE:HA	1:J:48:HIS:HD2	1.66	0.60
1:K:206:GLY:O	1:K:208:GLN:NE2	2.31	0.60
1:A:59:LEU:HA	1:B:345:LYS:HE3	1.84	0.59
1:E:252:PRO:O	1:E:255:VAL:HG23	2.02	0.59
1:H:28:ILE:HG22	1:H:30:SER:H	1.65	0.59
1:L:345:LYS:O	1:L:346:ASN:ND2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:130:ALA:O	1:J:135:LEU:N	2.31	0.59
1:G:255:VAL:HG21	1:H:121:HIS:NE2	2.16	0.59
1:K:126:LYS:HA	1:K:131:GLY:HA3	1.83	0.59
1:D:45:ASP:OD2	1:D:49:ARG:NE	2.35	0.59
1:E:219:TYR:HA	1:E:238:THR:HG22	1.85	0.59
1:G:236:ILE:HG21	1:G:246:ILE:HG12	1.85	0.59
1:H:348:LEU:HD21	1:H:361:GLY:HA3	1.85	0.59
1:I:53:GLY:O	1:I:58:ARG:NH1	2.36	0.59
1:K:271:ALA:HB3	1:L:6:VAL:HG21	1.84	0.59
1:E:356:SER:HB3	1:E:358:ASN:N	2.17	0.59
1:F:54:LEU:HB3	1:F:55:PRO:CD	2.32	0.59
1:G:10:ILE:HA	1:G:13:VAL:HB	1.85	0.59
1:G:43:ALA:HB2	1:H:43:ALA:HB2	1.85	0.59
1:G:85:HIS:NE2	1:G:247:ASP:OD1	2.28	0.59
1:I:50:TYR:HE2	1:I:256:SER:HB3	1.67	0.59
1:J:221:MET:HB2	1:J:236:ILE:HG12	1.84	0.59
1:I:105:THR:HG23	1:I:109:ASP:HB2	1.85	0.59
1:I:126:LYS:O	1:I:127:VAL:HG12	2.02	0.59
1:K:104:GLU:OE1	1:K:192:LYS:NZ	2.31	0.59
1:H:304:CYS:HB3	1:H:307:LYS:HB2	1.85	0.59
1:I:10:ILE:HA	1:I:13:VAL:HB	1.85	0.59
1:I:268:ILE:HD11	1:J:10:ILE:HD11	1.85	0.59
1:J:82:LYS:O	1:J:214:ARG:NH2	2.31	0.59
1:L:10:ILE:O	1:L:14:SER:N	2.36	0.59
1:E:101:PHE:O	1:E:105:THR:OG1	2.21	0.58
1:F:78:LYS:HB3	1:F:86:ALA:HB2	1.84	0.58
1:F:111:LEU:HB2	1:F:135:LEU:HD22	1.84	0.58
1:I:127:VAL:HG13	1:I:128:SER:N	2.17	0.58
1:L:26:LYS:HB2	1:L:368:GLU:OE1	2.03	0.58
1:B:251:PHE:CD1	1:B:252:PRO:CD	2.86	0.58
1:E:284:VAL:HG22	1:E:370:THR:HG21	1.83	0.58
1:G:176:PRO:HD3	1:G:209:PHE:CE1	2.39	0.58
1:E:52:GLU:HB3	1:E:251:PHE:CE1	2.38	0.58
1:F:162:LYS:HB3	1:F:163:PRO:HD3	1.85	0.58
1:K:24:SER:O	1:K:26:LYS:NZ	2.36	0.58
1:J:80:LEU:HD13	1:J:274:LEU:HA	1.83	0.58
1:J:95:VAL:HG22	1:J:99:ALA:HB2	1.85	0.58
1:A:111:LEU:HD21	1:A:167:LEU:HD12	1.84	0.58
1:F:115:SER:HB2	1:F:118:ASP:HB2	1.85	0.58
1:B:345:LYS:NZ	1:B:357:ASP:O	2.27	0.58
1:E:13:VAL:HG13	1:F:65:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:THR:HG23	1:G:228:PHE:H	1.68	0.58
1:H:53:GLY:HA3	1:H:258:HIS:NE2	2.18	0.58
1:I:90:PRO:HB3	1:I:95:VAL:HG12	1.85	0.58
1:K:172:LEU:HD23	1:K:363:ARG:HD3	1.86	0.58
1:C:280:TYR:HE1	1:C:371:ARG:HG2	1.68	0.58
1:D:261:HIS:HD1	1:D:261:HIS:H	1.50	0.58
1:E:289:LYS:CB	1:E:310:THR:HG22	2.31	0.58
1:J:345:LYS:NZ	1:J:357:ASP:OD2	2.33	0.58
1:K:167:LEU:HD23	1:K:194:ALA:HB3	1.85	0.58
1:B:82:LYS:HB2	1:B:214:ARG:HH22	1.69	0.58
1:D:23:GLU:HB3	1:D:404:LYS:HB2	1.86	0.58
1:G:183:TYR:HA	1:G:193:ILE:HD11	1.84	0.58
1:A:114:LEU:HD23	1:A:114:LEU:H	1.69	0.57
1:B:26:LYS:HA	1:B:342:ILE:HB	1.85	0.57
1:B:177:HIS:O	1:B:210:GLN:NE2	2.37	0.57
1:E:312:SER:OG	1:E:313:HIS:N	2.36	0.57
1:G:37:ALA:HB1	1:G:268:ILE:HD13	1.85	0.57
1:G:268:ILE:HD11	1:H:10:ILE:HD11	1.86	0.57
1:B:282:LYS:HG2	1:B:286:LYS:HE2	1.86	0.57
1:E:259:HIS:HB3	1:E:261:HIS:CE1	2.40	0.57
1:L:306:HIS:CD2	1:L:307:LYS:HG3	2.39	0.57
1:B:187:GLN:HG2	1:E:126:LYS:HE2	1.86	0.57
1:F:106:LYS:HA	1:F:133:ARG:HH12	1.69	0.57
1:G:30:SER:HB2	1:H:50:TYR:CD2	2.39	0.57
1:G:65:TYR:HB3	1:H:13:VAL:HG13	1.85	0.57
1:G:208:GLN:O	1:G:209:PHE:HB3	2.04	0.57
1:H:30:SER:OG	1:H:363:ARG:NH1	2.37	0.57
1:G:32:ASN:HD22	1:G:229:PHE:HA	1.69	0.57
1:G:18:HIS:HE1	1:G:39:ARG:HH22	1.51	0.57
1:K:25:ILE:HG12	1:K:341:ILE:HG22	1.87	0.57
1:L:19:GLU:HA	1:L:22:ARG:HE	1.69	0.57
1:A:354:ASN:HA	1:D:135:LEU:HD13	1.87	0.57
1:C:11:ARG:NH2	1:C:429:TYR:O	2.38	0.57
1:K:49:ARG:NH1	1:K:62:GLY:O	2.38	0.57
1:K:197:GLY:O	1:K:201:LEU:N	2.38	0.57
1:D:42:CYS:HA	1:D:261:HIS:HB2	1.86	0.57
1:G:313:HIS:HD2	1:G:367:GLN:HE21	1.52	0.57
1:I:306:HIS:CD2	1:I:307:LYS:HG2	2.40	0.57
1:J:357:ASP:O	1:J:359:PRO:HD3	2.04	0.57
1:G:227:THR:O	1:G:228:PHE:C	2.42	0.57
1:G:405:GLU:HA	1:G:408:LYS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:GLN:OE1	1:J:257:ASN:ND2	2.37	0.57
1:B:24:SER:O	1:B:26:LYS:NZ	2.38	0.57
1:I:111:LEU:HD21	1:I:167:LEU:HD12	1.86	0.57
1:K:238:THR:OG1	1:K:239:THR:N	2.37	0.57
1:E:196:ASP:HB2	1:E:221:MET:HE3	1.86	0.57
1:E:209:PHE:CE1	1:E:312:SER:HB2	2.39	0.57
1:F:7:PRO:O	1:F:10:ILE:HG13	2.05	0.57
1:G:268:ILE:O	1:G:272:GLU:HG2	2.05	0.57
1:I:319:ILE:HD11	1:I:362:ILE:HG12	1.87	0.57
1:J:24:SER:OG	1:J:340:ASN:ND2	2.33	0.57
1:L:223:SER:HB3	1:L:225:HIS:CD2	2.39	0.57
1:C:111:LEU:HD11	1:C:167:LEU:HG	1.87	0.56
1:G:30:SER:HB2	1:H:50:TYR:HD2	1.69	0.56
1:E:395:LYS:HE3	1:E:397:GLU:HB2	1.87	0.56
1:F:153:ALA:O	1:F:157:LYS:HB2	2.05	0.56
1:C:36:LEU:HB3	1:D:428:PHE:HB2	1.87	0.56
1:J:54:LEU:HB2	1:J:57:LYS:HG3	1.88	0.56
1:C:36:LEU:HD12	1:D:429:TYR:HB3	1.87	0.56
1:G:328:SER:HB3	1:G:358:ASN:HD21	1.70	0.56
1:G:428:PHE:HB3	1:H:36:LEU:HD22	1.87	0.56
1:F:249:HIS:O	1:F:253:GLY:HA3	2.06	0.56
1:G:54:LEU:HD12	1:G:55:PRO:HD2	1.88	0.56
1:I:119:GLY:HA2	1:I:172:LEU:HD13	1.86	0.56
1:K:101:PHE:O	1:K:105:THR:N	2.38	0.56
1:E:319:ILE:HG13	1:E:320:GLU:N	2.19	0.56
1:F:186:ALA:O	1:F:190:GLY:N	2.32	0.56
1:K:79:GLU:OE2	1:L:3:TYR:OH	2.23	0.56
1:L:175:PHE:HZ	1:L:307:LYS:HB3	1.71	0.56
1:A:271:ALA:HB3	1:B:6:VAL:HG21	1.86	0.56
1:F:295:LEU:HD21	1:F:317:ILE:HG13	1.87	0.56
1:H:25:ILE:HG13	1:H:403:VAL:HG13	1.87	0.56
1:A:48:HIS:HE1	1:B:39:ARG:HE	1.52	0.55
1:B:278:GLU:N	1:B:278:GLU:OE1	2.35	0.55
1:C:52:GLU:HB3	1:C:251:PHE:CZ	2.41	0.55
1:C:172:LEU:HD11	1:C:316:ILE:HG12	1.87	0.55
1:D:39:ARG:NH2	1:D:422:GLY:O	2.39	0.55
1:B:251:PHE:CB	1:B:252:PRO:HD3	2.30	0.55
1:D:246:ILE:O	1:D:250:VAL:HG12	2.06	0.55
1:F:74:ILE:HD13	1:F:88:VAL:HG13	1.87	0.55
1:F:83:ALA:HB2	1:F:213:LEU:HD13	1.88	0.55
1:H:211:ASP:OD1	1:H:214:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:ARG:O	1:J:59:LEU:HB2	2.07	0.55
1:J:204:ILE:HG21	1:J:220:LEU:HD11	1.88	0.55
1:L:47:MET:HG2	1:L:261:HIS:CG	2.42	0.55
1:D:36:LEU:HD11	1:D:422:GLY:HA2	1.87	0.55
1:F:368:GLU:HA	1:F:371:ARG:HB3	1.88	0.55
1:F:395:LYS:HZ2	1:F:397:GLU:H	1.53	0.55
1:I:45:ASP:HB2	1:J:18:HIS:CE1	2.41	0.55
1:I:239:THR:OG1	1:I:242:ASN:OD1	2.22	0.55
1:K:49:ARG:HD2	1:K:66:ILE:HD11	1.88	0.55
1:K:73:CYS:HB3	1:K:267:ALA:HB2	1.89	0.55
1:B:114:LEU:O	1:B:125:TRP:NE1	2.33	0.55
1:C:265:GLY:HA2	1:C:268:ILE:HD12	1.88	0.55
1:D:71:THR:O	1:D:75:GLU:HG2	2.06	0.55
1:D:107:PRO:HG3	1:D:133:ARG:HH12	1.70	0.55
1:G:72:LEU:HD21	1:H:6:VAL:HG13	1.89	0.55
1:L:104:GLU:O	1:L:105:THR:OG1	2.23	0.55
2:A:1430:PLP:O1P	1:B:256:SER:HB2	2.06	0.55
1:B:179:VAL:HG13	1:B:193:ILE:HG21	1.88	0.55
1:G:252:PRO:HB2	1:H:128:SER:HB3	1.88	0.55
1:I:23:GLU:HB3	1:I:404:LYS:HG2	1.88	0.55
1:I:112:MET:HB3	1:I:166:ILE:HA	1.87	0.55
1:D:119:GLY:O	1:D:171:SER:N	2.40	0.55
1:E:49:ARG:NH1	1:F:17:GLN:OE1	2.40	0.55
1:J:95:VAL:HB	1:J:254:VAL:HB	1.88	0.55
1:K:40:GLU:HB2	1:L:428:PHE:HB2	1.89	0.55
1:G:289:LYS:NZ	1:G:310:THR:O	2.29	0.55
1:B:245:LYS:O	1:B:249:HIS:ND1	2.39	0.55
1:E:259:HIS:HB2	1:E:262:HIS:HB2	1.88	0.55
1:I:25:ILE:HD11	1:I:403:VAL:HB	1.89	0.55
1:I:55:PRO:HG2	1:I:71:THR:HG23	1.88	0.55
1:K:127:VAL:O	1:L:252:PRO:HB2	2.07	0.55
1:A:236:ILE:HG21	1:A:246:ILE:HD13	1.89	0.55
1:D:34:THR:HG22	1:D:39:ARG:HH11	1.72	0.55
1:E:48:HIS:HB3	1:F:33:ILE:HA	1.89	0.55
1:J:199:HIS:HA	1:J:226:LYS:HG2	1.89	0.55
1:D:257:ASN:HB3	1:D:258:HIS:O	2.07	0.55
1:H:375:LYS:HG3	1:H:376:GLU:H	1.72	0.55
1:L:338:GLU:OE2	1:L:400:ARG:NH1	2.40	0.55
1:L:421:ASP:HB3	1:L:424:LYS:HB2	1.90	0.55
1:F:91:THR:O	1:F:233:GLY:HA2	2.07	0.54
1:F:52:GLU:HB3	1:F:251:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:GLY:H	1:I:177:HIS:CD2	2.25	0.54
1:B:34:THR:O	1:B:39:ARG:NH2	2.40	0.54
1:B:87:ASN:ND2	1:B:90:PRO:HD3	2.22	0.54
1:L:105:THR:HG23	1:L:109:ASP:HB2	1.89	0.54
1:L:345:LYS:HG2	1:L:359:PRO:HG3	1.90	0.54
1:A:48:HIS:CE1	1:B:39:ARG:HE	2.25	0.54
1:B:74:ILE:HD13	1:B:88:VAL:HG13	1.89	0.54
1:G:313:HIS:CD2	1:G:367:GLN:HE21	2.25	0.54
1:B:421:ASP:HB2	1:B:424:LYS:HG3	1.88	0.54
1:D:343:LEU:HB2	1:D:362:ILE:HD11	1.89	0.54
1:F:112:MET:HB3	1:F:166:ILE:HG23	1.90	0.54
1:G:31:GLU:HG2	1:H:50:TYR:H	1.71	0.54
1:L:52:GLU:OE1	1:L:58:ARG:NH1	2.41	0.54
1:L:193:ILE:HG23	1:L:218:GLU:H	1.72	0.54
1:A:29:ALA:O	1:A:367:GLN:NE2	2.41	0.54
1:B:351:ASP:CG	1:B:360:SER:H	2.10	0.54
1:F:387:LYS:HG3	1:F:391:ILE:HD12	1.89	0.54
1:C:376:GLU:O	1:C:379:MET:HG2	2.07	0.54
1:D:52:GLU:HG3	1:D:251:PHE:CZ	2.43	0.54
1:L:292:ALA:HB1	1:L:309:PHE:CD2	2.43	0.54
1:L:344:ASN:O	1:L:362:ILE:HG13	2.07	0.54
1:L:372:LEU:HA	1:L:413:ILE:HA	1.89	0.54
1:H:283:GLN:O	1:H:287:ASN:ND2	2.41	0.54
1:J:27:LEU:O	1:J:365:GLY:N	2.41	0.54
1:B:98:LEU:HB3	1:B:254:VAL:HG11	1.90	0.54
1:E:27:LEU:O	1:E:365:GLY:N	2.39	0.54
1:E:61:GLN:HB3	1:F:342:ILE:HG22	1.89	0.54
1:E:63:CYS:O	1:E:66:ILE:HG13	2.08	0.54
1:F:75:GLU:HA	1:F:78:LYS:HE2	1.90	0.54
1:I:48:HIS:CD2	1:J:34:THR:H	2.25	0.54
1:I:169:GLY:HA2	1:I:173:PHE:CE2	2.43	0.54
1:L:298:ARG:HG2	1:L:387:LYS:HG3	1.89	0.54
1:B:327:PHE:HB3	1:B:332:LEU:HG	1.90	0.53
1:L:27:LEU:O	1:L:365:GLY:N	2.38	0.53
1:A:46:PHE:HB3	1:A:260:LEU:HB2	1.89	0.53
1:B:80:LEU:HD11	1:B:205:ALA:HB1	1.89	0.53
1:E:344:ASN:HD21	1:F:60:TYR:HA	1.74	0.53
1:I:34:THR:H	1:J:48:HIS:CD2	2.25	0.53
1:A:133:ARG:NH1	1:B:131:GLY:O	2.42	0.53
1:C:40:GLU:CG	1:D:428:PHE:HD1	2.20	0.53
1:H:238:THR:HG21	1:H:246:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:GLU:OE1	1:I:305:GLU:N	2.37	0.53
1:A:13:VAL:HG13	1:B:65:TYR:HD1	1.73	0.53
1:B:218:GLU:OE2	1:B:242:ASN:ND2	2.40	0.53
1:B:251:PHE:HD1	1:B:252:PRO:HD3	1.73	0.53
1:C:48:HIS:CE1	1:D:33:ILE:HG13	2.43	0.53
1:C:148:ASN:ND2	1:C:176:PRO:O	2.41	0.53
1:E:128:SER:HA	1:F:252:PRO:O	2.08	0.53
1:F:102:PHE:HB3	1:F:249:HIS:HB3	1.90	0.53
1:F:107:PRO:HA	1:F:134:GLY:O	2.08	0.53
1:F:212:PRO:HA	1:F:215:GLU:HB2	1.90	0.53
1:L:89:GLN:N	1:L:90:PRO:HD2	2.24	0.53
1:A:240:LYS:HA	1:A:243:ALA:HB2	1.90	0.53
1:B:25:ILE:O	1:B:342:ILE:N	2.27	0.53
1:C:31:GLU:O	1:C:367:GLN:NE2	2.40	0.53
1:C:209:PHE:HE1	1:C:312:SER:HB3	1.74	0.53
1:D:52:GLU:HG2	1:D:53:GLY:N	2.24	0.53
1:G:416:SER:OG	1:G:418:ASP:O	2.24	0.53
1:H:126:LYS:O	1:H:127:VAL:HG22	2.08	0.53
1:I:105:THR:CG2	1:I:109:ASP:HB2	2.38	0.53
1:J:284:VAL:HG12	1:J:370:THR:HB	1.91	0.53
1:L:142:PHE:CD1	1:L:148:ASN:O	2.62	0.53
1:E:421:ASP:HB3	1:E:424:LYS:HB2	1.90	0.53
1:G:228:PHE:CD2	1:G:273:MET:HG3	2.44	0.53
1:G:412:THR:HA	1:G:420:GLY:O	2.08	0.53
1:I:209:PHE:CE1	1:I:312:SER:HB3	2.44	0.53
1:L:395:LYS:HB2	1:L:398:LYS:HG2	1.91	0.53
1:A:63:CYS:HA	1:A:66:ILE:HD12	1.90	0.53
1:G:128:SER:HA	1:H:253:GLY:HA3	1.91	0.53
1:G:176:PRO:HB2	1:G:210:GLN:NE2	2.24	0.53
1:K:168:PHE:CG	1:K:179:VAL:HG12	2.44	0.53
1:K:239:THR:OG1	1:K:242:ASN:OD1	2.21	0.53
1:G:32:ASN:ND2	1:G:227:THR:O	2.42	0.53
1:H:112:MET:HB2	1:H:163:PRO:HB2	1.91	0.53
1:J:140:HIS:HE1	1:J:166:ILE:HG23	1.73	0.53
1:K:35:SER:OG	1:K:371:ARG:NH2	2.41	0.53
1:K:45:ASP:O	1:K:48:HIS:HB2	2.09	0.53
1:C:298:ARG:HD2	1:C:387:LYS:HD3	1.91	0.53
1:C:328:SER:HB3	1:C:331:GLU:HG2	1.90	0.53
1:G:283:GLN:O	1:G:287:ASN:ND2	2.42	0.53
1:H:99:ALA:HA	1:H:254:VAL:HG21	1.91	0.53
1:J:159:LEU:O	1:J:162:LYS:NZ	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:303:LEU:HD11	1:L:350:TRP:HZ2	1.73	0.53
1:A:84:GLU:HB2	1:A:239:THR:HA	1.91	0.53
1:B:319:ILE:HG12	1:B:332:LEU:HD12	1.90	0.53
1:D:27:LEU:HD12	1:D:364:LEU:HB3	1.90	0.53
1:D:75:GLU:O	1:D:79:GLU:HG3	2.09	0.53
1:A:115:SER:O	1:A:120:GLY:N	2.36	0.52
1:C:251:PHE:O	1:C:251:PHE:CD2	2.62	0.52
1:D:325:ILE:HD12	1:D:390:ALA:HB1	1.89	0.52
1:G:147:MET:HG3	1:G:303:LEU:HD23	1.89	0.52
1:I:115:SER:HA	1:I:125:TRP:NE1	2.24	0.52
1:E:169:GLY:HA2	1:E:173:PHE:CE2	2.44	0.52
1:J:209:PHE:CE1	1:J:312:SER:HB3	2.45	0.52
1:K:94:VAL:HG11	1:L:254:VAL:HG13	1.91	0.52
1:D:201:LEU:HD22	1:D:222:GLY:HA3	1.91	0.52
1:D:381:GLU:O	1:D:384:GLU:HG2	2.09	0.52
1:J:87:ASN:ND2	1:J:247:ASP:OD1	2.42	0.52
1:G:325:ILE:HG21	1:G:390:ALA:HB1	1.91	0.52
1:H:80:LEU:HD21	1:H:205:ALA:HB1	1.90	0.52
1:I:48:HIS:HD2	1:J:33:ILE:HA	1.73	0.52
1:K:229:PHE:HB2	1:K:269:ALA:HB1	1.92	0.52
1:L:322:SER:OG	1:L:323:PRO:HD2	2.10	0.52
1:E:28:ILE:HG13	1:E:342:ILE:HG22	1.92	0.52
1:L:171:SER:OG	1:L:363:ARG:NH1	2.43	0.52
1:C:376:GLU:HA	1:C:379:MET:HE1	1.92	0.52
1:D:34:THR:CG2	1:D:39:ARG:HH11	2.23	0.52
1:G:229:PHE:HE1	1:G:272:GLU:HG3	1.74	0.52
1:I:58:ARG:NH2	1:I:70:GLU:OE1	2.31	0.52
1:K:236:ILE:HG21	1:K:246:ILE:HG12	1.92	0.52
1:K:268:ILE:HD11	1:L:10:ILE:HG12	1.90	0.52
1:A:10:ILE:O	1:A:14:SER:N	2.34	0.52
1:D:194:ALA:HA	1:D:219:TYR:HB2	1.92	0.52
1:D:245:LYS:O	1:D:249:HIS:ND1	2.39	0.52
1:D:315:VAL:HB	1:D:364:LEU:HB2	1.90	0.52
1:E:91:THR:O	1:E:233:GLY:HA2	2.10	0.52
1:E:280:TYR:O	1:E:284:VAL:HG23	2.10	0.52
1:I:329:ALA:HB1	1:I:362:ILE:HG23	1.90	0.52
1:J:224:THR:HG21	1:J:266:LEU:HD13	1.92	0.52
1:L:146:GLU:HG3	1:L:306:HIS:NE2	2.25	0.52
1:E:108:GLY:H	1:E:135:LEU:HD22	1.75	0.52
1:E:244:ASP:HA	1:E:247:ASP:HB2	1.91	0.52
1:G:421:ASP:HB3	1:G:424:LYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:340:ASN:OD1	1:K:400:ARG:NH1	2.43	0.52
1:A:195:TYR:HD2	1:A:220:LEU:HD13	1.75	0.52
1:C:199:HIS:O	1:C:227:THR:CG2	2.58	0.52
1:C:246:ILE:O	1:C:250:VAL:HG12	2.10	0.52
1:C:426:LEU:HB2	1:D:428:PHE:CE2	2.44	0.52
1:E:340:ASN:HB2	1:E:403:VAL:HG21	1.92	0.52
1:K:101:PHE:CD2	1:K:130:ALA:HB2	2.44	0.52
1:K:114:LEU:HD21	1:K:149:ILE:HD11	1.91	0.52
1:K:251:PHE:H	1:K:253:GLY:H	1.57	0.52
1:B:142:PHE:HB3	1:B:149:ILE:HA	1.92	0.52
1:D:429:TYR:OXT	1:K:392:ASP:HB3	2.10	0.52
1:E:243:ALA:O	1:E:246:ILE:HG22	2.10	0.52
1:H:315:VAL:HB	1:H:364:LEU:HB2	1.92	0.52
1:K:26:LYS:HE2	1:K:372:LEU:HD11	1.91	0.52
1:L:52:GLU:HB3	1:L:58:ARG:HA	1.92	0.52
1:C:297:GLU:OE2	1:C:298:ARG:NH2	2.43	0.51
1:F:22:ARG:NH2	1:F:421:ASP:OD2	2.42	0.51
1:F:352:ASP:OD1	1:F:352:ASP:N	2.43	0.51
1:B:247:ASP:HA	1:B:250:VAL:CG1	2.39	0.51
1:D:351:ASP:HB2	1:D:352:ASP:CG	2.25	0.51
1:F:339:ALA:HA	1:F:400:ARG:HG3	1.91	0.51
1:L:319:ILE:N	1:L:360:SER:O	2.32	0.51
1:D:351:ASP:C	1:D:352:ASP:OD1	2.49	0.51
1:E:142:PHE:O	1:E:144:PRO:HD3	2.10	0.51
1:G:232:GLN:HG3	1:H:261:HIS:HE1	1.76	0.51
1:I:115:SER:HB2	1:I:118:ASP:HB2	1.92	0.51
1:L:196:ASP:HA	1:L:221:MET:HG2	1.93	0.51
1:B:228:PHE:HZ	1:B:270:LEU:HD12	1.74	0.51
1:C:330:SER:HA	1:C:345:LYS:HD3	1.92	0.51
1:D:401:GLU:HA	1:D:404:LYS:HG2	1.93	0.51
1:F:106:LYS:N	1:F:109:ASP:OD2	2.39	0.51
1:L:319:ILE:O	1:L:325:ILE:HG21	2.11	0.51
1:D:143:ASP:HB3	1:D:146:GLU:O	2.10	0.51
1:E:240:LYS:HA	1:E:243:ALA:HB2	1.91	0.51
1:I:315:VAL:HB	1:I:364:LEU:HB2	1.92	0.51
1:D:209:PHE:CD2	1:D:210:GLN:HG2	2.46	0.51
1:E:158:ILE:HD12	1:E:185:ALA:HB3	1.93	0.51
1:E:296:TYR:HA	1:E:300:PHE:O	2.11	0.51
1:F:24:SER:O	1:F:26:LYS:NZ	2.32	0.51
1:F:251:PHE:HD2	1:F:252:PRO:HD3	1.75	0.51
1:I:199:HIS:O	1:I:227:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:LEU:HG	1:I:227:THR:HG21	1.92	0.51
1:I:343:LEU:HD13	1:I:362:ILE:HD13	1.92	0.51
1:I:357:ASP:N	1:I:357:ASP:OD1	2.44	0.51
1:K:130:ALA:O	1:K:135:LEU:N	2.42	0.51
1:K:23:GLU:HB3	1:K:404:LYS:HB2	1.91	0.51
1:K:45:ASP:HB2	1:L:18:HIS:CD2	2.46	0.51
1:L:113:ALA:HB2	1:L:167:LEU:HD12	1.91	0.51
1:B:28:ILE:HG22	1:B:30:SER:H	1.75	0.51
1:C:324:ASP:HB3	1:C:391:ILE:HG23	1.93	0.51
1:I:283:GLN:NE2	1:I:375:LYS:HD3	2.24	0.51
1:J:94:VAL:HG23	1:J:95:VAL:H	1.75	0.51
1:D:280:TYR:HE2	1:D:371:ARG:HD3	1.76	0.51
1:E:336:TYR:HE1	1:E:389:ILE:HB	1.76	0.51
1:G:25:ILE:HD11	1:G:341:ILE:HG23	1.93	0.51
1:J:27:LEU:HD22	1:J:364:LEU:HD22	1.92	0.51
1:J:250:VAL:HA	1:J:253:GLY:O	2.11	0.51
1:A:320:GLU:HB2	1:D:138:ILE:HD12	1.93	0.51
1:D:198:ALA:HA	1:D:223:SER:H	1.76	0.51
1:G:6:VAL:HG13	1:H:72:LEU:HD21	1.93	0.51
1:G:51:ALA:HB1	1:G:58:ARG:HH12	1.75	0.51
1:I:131:GLY:HA2	1:I:135:LEU:HG	1.93	0.51
1:I:229:PHE:CZ	1:I:273:MET:HB3	2.46	0.51
1:K:391:ILE:O	1:K:392:ASP:HB2	2.10	0.51
1:A:295:LEU:HG	1:A:300:PHE:HD2	1.75	0.50
1:B:379:MET:HA	1:B:382:ILE:HB	1.93	0.50
1:C:238:THR:OG1	1:C:239:THR:N	2.44	0.50
1:G:305:GLU:HA	1:G:309:PHE:CE1	2.46	0.50
1:H:251:PHE:HB3	1:H:252:PRO:HD3	1.93	0.50
1:L:47:MET:HG2	1:L:261:HIS:CD2	2.46	0.50
1:A:347:LEU:HG	1:A:359:PRO:HB3	1.93	0.50
1:E:304:CYS:HB3	1:E:307:LYS:HB2	1.93	0.50
1:H:42:CYS:HA	1:H:261:HIS:HB2	1.93	0.50
1:I:45:ASP:HB2	1:J:18:HIS:NE2	2.26	0.50
1:L:66:ILE:HA	1:L:69:VAL:HG12	1.92	0.50
1:E:110:LYS:HB3	1:E:163:PRO:HA	1.93	0.50
1:J:141:PRO:HB2	1:J:150:ASP:HB3	1.93	0.50
1:J:224:THR:HG22	1:J:230:GLY:HA3	1.92	0.50
1:B:283:GLN:HG2	1:B:375:LYS:HZ3	1.77	0.50
1:C:132:ILE:HG23	1:D:133:ARG:HD2	1.92	0.50
1:C:199:HIS:O	1:C:227:THR:HG23	2.12	0.50
1:G:18:HIS:CE1	1:G:39:ARG:HH22	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:HG3	1:H:5:ASP:HB2	1.93	0.50
1:J:140:HIS:CE1	1:J:166:ILE:HG23	2.46	0.50
1:L:53:GLY:HA2	1:L:89:GLN:HE22	1.75	0.50
1:L:371:ARG:O	1:L:414:HIS:N	2.43	0.50
1:A:269:ALA:HA	1:A:272:GLU:HB2	1.94	0.50
1:D:285:ILE:HG13	1:D:311:GLU:O	2.11	0.50
1:K:48:HIS:NE2	1:L:368:GLU:OE1	2.42	0.50
1:L:146:GLU:HB3	1:L:307:LYS:NZ	2.26	0.50
1:B:251:PHE:CB	1:B:252:PRO:CD	2.87	0.50
1:C:146:GLU:HG3	1:C:306:HIS:CE1	2.46	0.50
1:G:401:GLU:HA	1:G:404:LYS:HD3	1.94	0.50
1:J:94:VAL:HG23	1:J:95:VAL:N	2.27	0.50
1:A:50:TYR:CD2	1:B:30:SER:CB	2.90	0.50
1:D:162:LYS:HG3	1:D:189:VAL:HG22	1.94	0.50
1:D:388:ARG:HH22	1:I:375:LYS:HD2	1.76	0.50
1:I:280:TYR:O	1:I:284:VAL:HG23	2.12	0.50
1:B:6:VAL:HG23	1:B:7:PRO:HD3	1.93	0.50
1:F:259:HIS:HB3	1:F:261:HIS:CE1	2.47	0.50
1:H:346:ASN:OD1	1:H:363:ARG:HB2	2.12	0.50
1:I:51:ALA:HB2	1:I:66:ILE:HG21	1.93	0.50
1:A:175:PHE:CD1	1:A:310:THR:OG1	2.53	0.50
1:C:58:ARG:NH2	1:C:70:GLU:OE1	2.45	0.50
1:E:251:PHE:O	1:E:251:PHE:CG	2.64	0.50
1:J:333:ALA:HA	1:J:343:LEU:HD11	1.92	0.50
1:L:295:LEU:HD12	1:L:387:LYS:NZ	2.27	0.50
1:B:193:ILE:HB	1:B:217:ALA:HA	1.92	0.49
1:C:81:PHE:O	1:C:214:ARG:NH2	2.45	0.49
1:F:112:MET:HE1	1:F:157:LYS:HG2	1.94	0.49
1:I:126:LYS:HE2	1:I:135:LEU:HB3	1.94	0.49
1:I:129:ALA:H	1:I:132:ILE:HG13	1.77	0.49
1:J:223:SER:HB2	1:J:225:HIS:CE1	2.46	0.49
1:D:197:GLY:O	1:D:201:LEU:N	2.43	0.49
1:D:209:PHE:CE1	1:D:312:SER:HB3	2.48	0.49
1:E:259:HIS:O	1:E:263:LYS:HG2	2.12	0.49
1:G:63:CYS:O	1:G:64:LYS:HD2	2.11	0.49
1:A:213:LEU:HB2	1:A:214:ARG:NH1	2.27	0.49
1:B:298:ARG:HH21	1:B:380:GLU:HG3	1.77	0.49
1:F:186:ALA:HB1	1:F:191:ALA:O	2.12	0.49
1:F:199:HIS:HA	1:F:226:LYS:HD2	1.93	0.49
1:F:287:ASN:HB3	1:F:379:MET:HE1	1.94	0.49
1:F:312:SER:OG	1:F:313:HIS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:ASP:HB3	1:J:136:LYS:N	2.26	0.49
1:K:135:LEU:HD13	1:L:133:ARG:NH1	2.27	0.49
1:A:10:ILE:HD11	1:B:268:ILE:HD11	1.94	0.49
1:B:389:ILE:HA	1:B:394:GLU:HB3	1.93	0.49
1:E:291:LEU:O	1:E:295:LEU:HB2	2.13	0.49
1:G:122:ILE:O	1:G:123:SER:OG	2.29	0.49
1:I:255:VAL:HG22	1:I:256:SER:H	1.78	0.49
1:K:223:SER:HB2	1:K:225:HIS:CE1	2.47	0.49
1:B:63:CYS:HA	1:B:66:ILE:HD13	1.94	0.49
1:D:28:ILE:HB	1:D:31:GLU:HG2	1.94	0.49
1:D:294:ALA:O	1:D:298:ARG:HG2	2.13	0.49
1:F:110:LYS:HE2	1:F:136:LYS:HD2	1.94	0.49
1:G:146:GLU:HG2	1:G:306:HIS:NE2	2.27	0.49
1:J:70:GLU:OE2	1:J:89:GLN:NE2	2.44	0.49
1:K:225:HIS:ND1	1:K:232:GLN:HA	2.28	0.49
1:K:280:TYR:O	1:K:284:VAL:HG23	2.13	0.49
1:K:304:CYS:HB3	1:K:307:LYS:HD2	1.93	0.49
1:A:110:LYS:NZ	1:C:241:GLU:OE1	2.41	0.49
1:C:103:ALA:HA	1:C:249:HIS:CD2	2.47	0.49
1:E:36:LEU:HD12	1:E:39:ARG:HH12	1.77	0.49
1:E:154:MET:HA	1:E:157:LYS:NZ	2.28	0.49
1:E:395:LYS:HD2	1:E:396:PRO:HD2	1.94	0.49
1:F:248:SER:O	1:F:252:PRO:HD2	2.12	0.49
1:L:112:MET:O	1:L:167:LEU:N	2.45	0.49
1:L:203:LEU:HD13	1:L:227:THR:HB	1.95	0.49
1:C:7:PRO:HG3	1:D:417:PHE:CD2	2.48	0.49
1:D:178:PRO:HB2	1:D:181:ASP:HB2	1.93	0.49
1:F:245:LYS:O	1:F:249:HIS:ND1	2.43	0.49
1:G:378:GLU:HG2	1:G:410:TYR:OH	2.12	0.49
1:H:27:LEU:HB2	1:H:342:ILE:O	2.12	0.49
1:H:91:THR:H	1:H:95:VAL:HG11	1.77	0.49
1:I:49:ARG:NH1	1:J:21:MET:HG3	2.28	0.49
1:I:112:MET:HG3	1:I:140:HIS:CE1	2.48	0.49
1:J:51:ALA:HB2	1:J:260:LEU:HD11	1.94	0.49
1:C:176:PRO:HB3	1:C:210:GLN:HB2	1.95	0.49
2:C:1430:PLP:O1P	1:D:255:VAL:HG22	2.12	0.49
1:E:157:LYS:HB3	1:E:157:LYS:HE2	1.49	0.49
1:H:238:THR:OG1	1:H:239:THR:N	2.45	0.49
1:I:330:SER:OG	1:I:358:ASN:OD1	2.26	0.49
1:J:176:PRO:HB3	1:J:210:GLN:HB2	1.93	0.49
1:K:165:LEU:HD13	1:K:192:LYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:HIS:HA	1:K:226:LYS:HD2	1.94	0.49
1:K:355:ASN:OD1	1:K:355:ASN:N	2.46	0.49
1:B:345:LYS:HD2	1:B:359:PRO:HD2	1.95	0.49
1:A:288:ALA:HA	1:A:366:THR:HG21	1.95	0.48
1:C:59:LEU:HA	1:D:345:LYS:HD3	1.94	0.48
1:C:369:CYS:O	1:C:374:MET:HB2	2.13	0.48
1:D:32:ASN:HA	1:D:368:GLU:HB2	1.94	0.48
1:E:416:SER:OG	1:E:417:PHE:N	2.46	0.48
1:F:197:GLY:O	1:F:201:LEU:N	2.46	0.48
1:G:175:PHE:CD1	1:G:311:GLU:HG2	2.47	0.48
1:H:388:ARG:HA	1:H:392:ASP:HB2	1.94	0.48
1:I:31:GLU:OE1	1:J:49:ARG:NH1	2.46	0.48
1:L:76:LEU:HD12	1:L:274:LEU:HD11	1.95	0.48
1:L:225:HIS:CE1	1:L:232:GLN:HG3	2.48	0.48
1:L:305:GLU:H	1:L:305:GLU:CD	2.16	0.48
1:A:369:CYS:HB3	1:A:379:MET:HE1	1.95	0.48
1:C:287:ASN:HA	1:C:379:MET:CE	2.43	0.48
1:F:73:CYS:HB3	1:F:88:VAL:HG11	1.94	0.48
1:G:78:LYS:O	1:G:82:LYS:N	2.47	0.48
1:H:167:LEU:HD23	1:H:194:ALA:HB3	1.94	0.48
1:J:305:GLU:H	1:J:305:GLU:CD	2.15	0.48
1:A:47:MET:HB2	1:A:261:HIS:CG	2.48	0.48
1:E:43:ALA:HB2	1:F:43:ALA:HB2	1.95	0.48
1:G:175:PHE:HD1	1:G:311:GLU:HG2	1.79	0.48
1:G:345:LYS:HA	1:G:362:ILE:HD13	1.95	0.48
1:H:169:GLY:HA2	1:H:173:PHE:CE2	2.48	0.48
1:H:245:LYS:O	1:H:249:HIS:ND1	2.45	0.48
1:I:102:PHE:CZ	1:J:127:VAL:HA	2.48	0.48
1:J:126:LYS:O	1:J:127:VAL:HG22	2.13	0.48
1:J:148:ASN:OD1	1:J:149:ILE:N	2.46	0.48
1:J:348:LEU:HD13	1:J:361:GLY:HA3	1.94	0.48
1:B:345:LYS:HA	1:B:362:ILE:HD13	1.95	0.48
1:F:162:LYS:HB3	1:F:163:PRO:CD	2.42	0.48
1:G:34:THR:H	1:H:48:HIS:CE1	2.31	0.48
1:A:27:LEU:HB2	1:A:343:LEU:HB3	1.96	0.48
1:D:89:GLN:HG2	1:D:258:HIS:NE2	2.28	0.48
1:F:72:LEU:O	1:F:76:LEU:HB2	2.13	0.48
1:F:105:THR:O	1:F:133:ARG:NH1	2.45	0.48
1:H:32:ASN:ND2	1:H:227:THR:O	2.46	0.48
1:I:38:VAL:HG13	1:I:265:GLY:HA3	1.93	0.48
1:I:231:PRO:HB2	1:I:262:HIS:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:371:ARG:NH2	1:J:415:TYR:O	2.46	0.48
1:K:342:ILE:HG21	1:L:62:GLY:HA3	1.95	0.48
1:A:62:GLY:HA2	1:B:20:TRP:CH2	2.48	0.48
1:C:62:GLY:O	1:C:66:ILE:HD13	2.13	0.48
1:C:319:ILE:HD13	1:C:332:LEU:HD23	1.96	0.48
1:G:32:ASN:O	1:H:48:HIS:HB3	2.13	0.48
1:G:228:PHE:CE2	1:G:273:MET:HG3	2.48	0.48
1:G:272:GLU:OE2	1:G:371:ARG:NH2	2.45	0.48
1:H:32:ASN:ND2	1:H:367:GLN:HB2	2.29	0.48
1:H:37:ALA:HB1	1:H:268:ILE:HD13	1.95	0.48
1:H:227:THR:O	1:H:228:PHE:C	2.52	0.48
1:A:303:LEU:HD11	1:A:348:LEU:HD13	1.96	0.48
1:D:281:ALA:O	1:D:285:ILE:HG22	2.14	0.48
1:E:354:ASN:OD1	1:E:354:ASN:N	2.44	0.48
1:G:50:TYR:CE1	1:G:257:ASN:HB2	2.48	0.48
1:H:271:ALA:HA	1:H:274:LEU:HD12	1.94	0.48
1:I:105:THR:HG22	1:I:106:LYS:O	2.13	0.48
1:I:287:ASN:ND2	1:I:374:MET:O	2.45	0.48
1:K:146:GLU:HG3	1:K:307:LYS:NZ	2.29	0.48
1:B:94:VAL:HG13	2:B:1430:PLP:O2P	2.13	0.48
1:C:94:VAL:HG21	1:D:255:VAL:HA	1.95	0.48
1:C:169:GLY:HA2	1:C:173:PHE:CE1	2.49	0.48
1:D:427:ARG:NH1	1:K:392:ASP:OD1	2.47	0.48
1:I:228:PHE:HA	1:I:273:MET:HE1	1.95	0.48
1:L:291:LEU:HD13	1:L:379:MET:HB3	1.95	0.48
1:B:115:SER:HB2	1:B:118:ASP:HB2	1.95	0.48
1:E:46:PHE:HB3	1:E:260:LEU:CB	2.44	0.48
1:F:377:LYS:O	1:F:380:GLU:HB3	2.13	0.48
1:I:122:ILE:C	1:I:124:HIS:H	2.17	0.48
1:L:41:ALA:O	1:L:44:THR:OG1	2.27	0.48
1:A:339:ALA:O	1:A:403:VAL:HG11	2.13	0.48
1:C:70:GLU:O	1:C:74:ILE:HG12	2.14	0.48
1:D:36:LEU:O	1:D:40:GLU:HG3	2.14	0.48
1:D:285:ILE:HG23	1:D:286:LYS:HD2	1.95	0.48
1:F:317:ILE:HB	1:F:362:ILE:HG13	1.95	0.48
1:G:32:ASN:HA	1:G:368:GLU:HB2	1.95	0.48
1:J:73:CYS:HB3	1:J:88:VAL:HG11	1.96	0.48
1:L:63:CYS:O	1:L:66:ILE:N	2.46	0.48
1:L:244:ASP:HA	1:L:247:ASP:HB2	1.96	0.48
1:L:251:PHE:CZ	1:L:258:HIS:HB2	2.49	0.48
1:A:227:THR:HG22	1:A:227:THR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HD3	1:B:368:GLU:HG3	1.96	0.47
1:C:114:LEU:O	1:C:125:TRP:NE1	2.43	0.47
1:C:157:LYS:O	1:C:161:GLU:HB2	2.14	0.47
1:D:140:HIS:CG	1:D:149:ILE:HG12	2.49	0.47
1:D:225:HIS:CD2	1:D:232:GLN:HG3	2.49	0.47
1:E:105:THR:C	1:E:133:ARG:HH12	2.18	0.47
1:K:44:THR:HG21	1:L:14:SER:HB3	1.96	0.47
1:A:126:LYS:O	1:A:127:VAL:HG22	2.15	0.47
1:A:162:LYS:HG2	1:A:189:VAL:HG13	1.96	0.47
1:E:348:LEU:HD11	1:E:361:GLY:HA3	1.96	0.47
1:F:203:LEU:HD13	1:F:285:ILE:HD11	1.95	0.47
1:G:13:VAL:HG13	1:H:65:TYR:HB3	1.96	0.47
1:J:210:GLN:NE2	1:J:215:GLU:OE1	2.43	0.47
1:K:202:GLY:HA3	1:K:227:THR:O	2.13	0.47
1:K:421:ASP:HB3	1:K:424:LYS:HB2	1.96	0.47
1:C:344:ASN:HD21	1:C:363:ARG:HE	1.60	0.47
1:D:225:HIS:HD2	1:D:233:GLY:H	1.60	0.47
1:G:176:PRO:HB2	1:G:210:GLN:HE21	1.80	0.47
1:I:115:SER:HA	1:I:125:TRP:HE1	1.79	0.47
1:I:292:ALA:HB1	1:I:302:VAL:HG11	1.95	0.47
1:L:310:THR:OG1	1:L:312:SER:N	2.38	0.47
1:L:319:ILE:HG21	1:L:329:ALA:HA	1.96	0.47
1:B:165:LEU:HD11	1:B:194:ALA:HB2	1.97	0.47
1:C:52:GLU:O	1:C:58:ARG:HB2	2.13	0.47
1:C:133:ARG:NH1	1:D:131:GLY:O	2.43	0.47
1:D:250:VAL:HG23	1:D:254:VAL:HB	1.96	0.47
1:G:176:PRO:HD3	1:G:209:PHE:HE1	1.77	0.47
1:J:176:PRO:HD3	1:J:209:PHE:CE1	2.49	0.47
1:K:305:GLU:OE1	1:K:305:GLU:N	2.45	0.47
1:D:300:PHE:CZ	1:D:390:ALA:HB3	2.47	0.47
1:F:379:MET:HA	1:F:382:ILE:HB	1.96	0.47
1:G:99:ALA:HB1	1:G:250:VAL:HG22	1.96	0.47
1:H:45:ASP:C	1:H:47:MET:H	2.17	0.47
1:H:199:HIS:O	1:H:227:THR:OG1	2.29	0.47
1:I:95:VAL:HG13	1:I:254:VAL:HG21	1.97	0.47
1:K:199:HIS:O	1:K:227:THR:OG1	2.25	0.47
1:K:259:HIS:ND1	1:L:232:GLN:HG2	2.29	0.47
1:A:132:ILE:HG22	1:B:132:ILE:HG22	1.96	0.47
1:A:246:ILE:HA	1:A:249:HIS:HB2	1.97	0.47
1:A:259:HIS:HB2	1:A:262:HIS:HB2	1.97	0.47
1:D:108:GLY:HA2	1:D:135:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:VAL:HG21	1:E:221:MET:SD	2.54	0.47
1:J:178:PRO:HB2	1:J:181:ASP:HB2	1.97	0.47
1:B:366:THR:O	1:B:370:THR:N	2.40	0.47
1:C:130:ALA:O	1:C:135:LEU:N	2.48	0.47
1:C:418:ASP:HB2	1:D:429:TYR:CG	2.50	0.47
1:D:22:ARG:NE	1:D:411:SER:HB2	2.30	0.47
1:F:112:MET:HG2	1:F:140:HIS:CE1	2.49	0.47
1:G:31:GLU:HG2	1:H:50:TYR:N	2.29	0.47
1:G:66:ILE:HG22	1:G:260:LEU:HD22	1.95	0.47
1:G:88:VAL:O	1:G:263:LYS:NZ	2.27	0.47
1:G:312:SER:OG	1:G:313:HIS:N	2.47	0.47
1:H:206:GLY:O	1:H:208:GLN:NE2	2.38	0.47
1:H:294:ALA:O	1:H:298:ARG:HG2	2.15	0.47
1:I:102:PHE:HZ	1:J:127:VAL:HA	1.79	0.47
1:I:110:LYS:HE2	1:I:136:LYS:NZ	2.30	0.47
1:I:132:ILE:HA	1:J:133:ARG:HD3	1.96	0.47
1:I:146:GLU:HA	1:I:304:CYS:SG	2.55	0.47
1:I:325:ILE:HG22	1:I:327:PHE:HB2	1.97	0.47
1:J:95:VAL:HA	1:J:98:LEU:HB2	1.97	0.47
1:K:411:SER:HB2	1:K:421:ASP:OD1	2.14	0.47
1:L:181:ASP:OD1	1:L:181:ASP:N	2.47	0.47
1:L:202:GLY:HA3	1:L:227:THR:O	2.15	0.47
1:L:305:GLU:HA	1:L:309:PHE:CE1	2.50	0.47
1:B:23:GLU:HG3	1:B:340:ASN:ND2	2.30	0.47
1:F:58:ARG:HH21	1:F:67:ASP:HA	1.80	0.47
1:G:32:ASN:ND2	1:G:229:PHE:HA	2.29	0.47
1:I:123:SER:HA	1:I:128:SER:O	2.15	0.47
1:A:126:LYS:HA	1:A:131:GLY:HA3	1.95	0.47
1:D:149:ILE:H	1:D:149:ILE:HD12	1.79	0.47
1:D:163:PRO:HG2	1:D:166:ILE:HD11	1.97	0.47
1:F:51:ALA:O	1:F:58:ARG:HD2	2.15	0.47
1:F:53:GLY:HA2	1:F:251:PHE:CE1	2.50	0.47
1:H:101:PHE:CD2	1:H:130:ALA:HB2	2.50	0.47
1:J:53:GLY:O	1:J:89:GLN:NE2	2.45	0.47
1:J:155:VAL:HG13	1:J:185:ALA:HB1	1.96	0.47
1:A:121:HIS:HB2	1:A:171:SER:HB3	1.97	0.47
1:B:315:VAL:HB	1:B:364:LEU:HB2	1.97	0.47
1:E:92:SER:O	1:E:95:VAL:HG22	2.15	0.47
1:F:238:THR:OG1	1:F:239:THR:N	2.48	0.47
1:F:339:ALA:O	1:F:341:ILE:N	2.48	0.47
1:I:318:ASP:OD1	1:I:360:SER:OG	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:LEU:HD11	1:J:194:ALA:HB2	1.97	0.47
1:J:232:GLN:HB2	1:J:262:HIS:CE1	2.50	0.47
1:K:78:LYS:HE2	1:K:86:ALA:N	2.29	0.47
1:B:118:ASP:HB3	1:B:142:PHE:HE1	1.80	0.46
1:C:127:VAL:HG13	1:D:252:PRO:HG2	1.97	0.46
1:G:81:PHE:HB2	1:G:237:LEU:HD22	1.98	0.46
1:G:169:GLY:HA2	1:G:173:PHE:CE2	2.50	0.46
1:J:5:ASP:OD1	1:J:5:ASP:N	2.42	0.46
1:D:405:GLU:HB3	1:I:286:LYS:NZ	2.30	0.46
1:G:47:MET:HA	1:G:261:HIS:HD2	1.79	0.46
1:G:47:MET:O	1:H:232:GLN:NE2	2.49	0.46
1:G:50:TYR:CE2	1:H:30:SER:HB3	2.49	0.46
1:G:336:TYR:HB3	1:G:341:ILE:O	2.15	0.46
1:A:174:PRO:O	1:A:310:THR:OG1	2.34	0.46
1:A:268:ILE:HD11	1:B:10:ILE:HD11	1.97	0.46
1:C:290:ALA:HB3	1:C:379:MET:CE	2.45	0.46
1:E:72:LEU:HD13	1:E:267:ALA:HB1	1.95	0.46
1:G:223:SER:OG	2:G:1430:PLP:O1P	2.33	0.46
1:H:106:LYS:N	1:H:109:ASP:OD2	2.42	0.46
1:J:154:MET:HG3	1:J:155:VAL:H	1.80	0.46
1:A:101:PHE:CE1	1:A:167:LEU:HD11	2.50	0.46
1:B:238:THR:OG1	1:B:239:THR:N	2.47	0.46
1:E:82:LYS:HB2	1:E:214:ARG:NH2	2.30	0.46
1:E:141:PRO:HG3	1:E:157:LYS:HD3	1.97	0.46
1:F:102:PHE:HD1	1:F:133:ARG:HH21	1.62	0.46
1:I:328:SER:HB3	1:I:331:GLU:HG2	1.96	0.46
1:J:143:ASP:HB3	1:J:146:GLU:O	2.16	0.46
1:D:49:ARG:HB2	1:D:260:LEU:HD12	1.97	0.46
1:D:174:PRO:O	1:D:311:GLU:N	2.47	0.46
1:E:158:ILE:HG22	1:E:189:VAL:HG21	1.97	0.46
1:F:58:ARG:HH22	1:F:70:GLU:CD	2.19	0.46
1:F:111:LEU:HB2	1:F:135:LEU:CD2	2.45	0.46
1:H:28:ILE:HG23	1:H:363:ARG:HD2	1.97	0.46
1:H:72:LEU:O	1:H:76:LEU:HB2	2.16	0.46
1:I:51:ALA:HB3	1:I:258:HIS:NE2	2.30	0.46
1:B:1:MET:HG2	1:B:5:ASP:OD1	2.15	0.46
1:C:102:PHE:CD1	1:D:132:ILE:HG12	2.50	0.46
1:C:306:HIS:HB3	1:E:306:HIS:HB3	1.98	0.46
1:D:336:TYR:CD2	1:D:343:LEU:HD21	2.51	0.46
1:G:140:HIS:CG	1:G:149:ILE:HD12	2.50	0.46
1:I:303:LEU:HD21	1:I:350:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:THR:OG1	1:J:239:THR:N	2.49	0.46
1:K:155:VAL:O	1:K:159:LEU:HB2	2.16	0.46
1:K:393:LYS:HE2	1:K:393:LYS:HB3	1.64	0.46
1:A:91:THR:HG23	1:A:255:VAL:HG23	1.96	0.46
1:B:46:PHE:HB3	1:B:260:LEU:HB3	1.98	0.46
1:B:376:GLU:HA	1:B:379:MET:HE2	1.97	0.46
1:C:135:LEU:HB3	1:C:136:LYS:H	1.55	0.46
1:E:371:ARG:NH2	1:E:416:SER:HB2	2.30	0.46
1:F:105:THR:HG22	1:F:133:ARG:NH1	2.31	0.46
1:H:32:ASN:HB2	1:H:367:GLN:HG3	1.98	0.46
1:I:55:PRO:HG3	1:I:58:ARG:HH21	1.80	0.46
1:D:214:ARG:HH11	1:D:214:ARG:H	1.63	0.46
1:D:225:HIS:CG	1:D:232:GLN:HG3	2.51	0.46
1:E:198:ALA:HA	1:E:223:SER:H	1.81	0.46
1:G:294:ALA:O	1:G:298:ARG:HG2	2.15	0.46
1:H:27:LEU:HD22	1:H:343:LEU:HD22	1.98	0.46
1:H:49:ARG:HA	1:H:49:ARG:HD3	1.72	0.46
1:I:169:GLY:HA2	1:I:173:PHE:HE2	1.80	0.46
1:J:227:THR:HG22	1:J:367:GLN:HG2	1.98	0.46
1:K:132:ILE:HD13	1:L:98:LEU:HD11	1.97	0.46
1:B:26:LYS:HB2	1:B:368:GLU:HG2	1.98	0.46
1:D:136:LYS:HD3	1:D:136:LYS:HA	1.73	0.46
1:E:150:ASP:OD1	1:E:153:ALA:N	2.46	0.46
1:G:36:LEU:HD21	1:G:421:ASP:H	1.81	0.46
1:H:246:ILE:O	1:H:250:VAL:HG23	2.15	0.46
1:J:97:ASN:HB3	1:J:101:PHE:CE2	2.51	0.46
1:J:367:GLN:H	1:J:367:GLN:HG3	1.55	0.46
1:A:50:TYR:HD2	1:B:30:SER:HB3	1.75	0.46
1:A:246:ILE:O	1:A:250:VAL:HG22	2.15	0.46
1:C:57:LYS:NZ	1:C:61:GLN:HA	2.31	0.46
1:D:226:LYS:C	1:D:228:PHE:H	2.19	0.46
1:F:81:PHE:HB2	1:F:237:LEU:HD22	1.98	0.46
1:F:117:PRO:HA	1:F:347:LEU:HB3	1.98	0.46
1:I:39:ARG:NH2	1:I:424:LYS:O	2.49	0.46
1:I:122:ILE:HG22	1:I:123:SER:H	1.80	0.46
1:I:319:ILE:HB	1:I:329:ALA:HB2	1.97	0.46
1:K:428:PHE:N	1:L:40:GLU:OE2	2.44	0.46
1:C:34:THR:HG23	1:D:48:HIS:CD2	2.52	0.45
1:D:336:TYR:HA	1:D:339:ALA:HB3	1.96	0.45
1:E:257:ASN:OD1	1:E:257:ASN:N	2.50	0.45
1:F:106:LYS:NZ	1:F:109:ASP:OD1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:MET:O	1:F:158:ILE:HG13	2.16	0.45
1:G:10:ILE:HD12	1:H:267:ALA:HB3	1.98	0.45
1:I:36:LEU:HD13	1:I:422:GLY:HA2	1.98	0.45
1:L:91:THR:H	1:L:95:VAL:HG11	1.81	0.45
1:A:267:ALA:HA	1:A:270:LEU:HD12	1.98	0.45
1:C:388:ARG:HD3	1:C:394:GLU:HG3	1.98	0.45
1:D:52:GLU:HB3	1:D:60:TYR:HE2	1.80	0.45
1:D:84:GLU:HB2	1:D:239:THR:HA	1.99	0.45
1:E:40:GLU:HB2	1:F:428:PHE:HB2	1.98	0.45
1:G:301:ASN:O	1:G:317:ILE:HG23	2.15	0.45
1:H:54:LEU:HD23	1:H:54:LEU:HA	1.86	0.45
1:I:377:LYS:O	1:I:381:GLU:HG2	2.17	0.45
1:A:10:ILE:HG13	1:A:11:ARG:N	2.31	0.45
1:C:69:VAL:HG11	1:C:264:ALA:HA	1.98	0.45
1:C:94:VAL:HB	1:D:255:VAL:HG23	1.98	0.45
1:C:209:PHE:CE1	1:C:312:SER:HB3	2.52	0.45
1:D:254:VAL:HG13	1:D:255:VAL:N	2.31	0.45
1:E:156:LYS:HA	1:E:159:LEU:HD12	1.97	0.45
1:E:165:LEU:HD21	1:E:194:ALA:HB3	1.97	0.45
1:F:63:CYS:HA	1:F:66:ILE:HD12	1.99	0.45
1:G:347:LEU:HD11	1:G:354:ASN:HA	1.97	0.45
1:J:93:GLY:N	2:J:1430:PLP:O1P	2.49	0.45
1:J:110:LYS:HE2	1:J:161:GLU:HB2	1.99	0.45
1:K:33:ILE:HB	1:K:368:GLU:HG3	1.99	0.45
1:K:109:ASP:HA	1:K:136:LYS:HB3	1.98	0.45
1:K:259:HIS:O	1:K:263:LYS:HG2	2.16	0.45
1:L:52:GLU:H	1:L:58:ARG:HG2	1.81	0.45
1:C:72:LEU:HD11	1:D:9:PHE:CD2	2.51	0.45
1:G:352:ASP:HB3	1:J:136:LYS:CA	2.47	0.45
1:J:173:PHE:HE1	1:J:177:HIS:CE1	2.33	0.45
1:K:126:LYS:HE3	1:K:135:LEU:HD12	1.98	0.45
1:K:169:GLY:HA2	1:K:173:PHE:CE2	2.52	0.45
1:L:383:ALA:O	1:L:387:LYS:HG2	2.16	0.45
1:C:225:HIS:HE1	1:D:50:TYR:CE2	2.34	0.45
1:C:322:SER:HA	1:C:323:PRO:HD3	1.75	0.45
1:C:378:GLU:OE2	1:C:410:TYR:OH	2.33	0.45
1:C:428:PHE:CD1	1:D:40:GLU:HG2	2.52	0.45
1:E:84:GLU:OE1	1:E:240:LYS:HG2	2.17	0.45
1:F:339:ALA:HB2	1:F:396:PRO:O	2.15	0.45
1:G:34:THR:HG23	1:H:48:HIS:ND1	2.32	0.45
1:I:20:TRP:CZ3	1:J:62:GLY:HA2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:CYS:HA	1:I:261:HIS:HB2	1.98	0.45
1:I:126:LYS:HE2	1:I:136:LYS:H	1.81	0.45
1:J:253:GLY:O	1:J:255:VAL:N	2.50	0.45
1:K:14:SER:O	1:K:17:GLN:HB3	2.16	0.45
1:K:49:ARG:HA	1:L:31:GLU:CD	2.37	0.45
1:K:138:ILE:HG21	1:K:157:LYS:NZ	2.31	0.45
1:L:95:VAL:HG13	1:L:254:VAL:HG21	1.99	0.45
1:L:174:PRO:HB3	1:L:316:ILE:HD11	1.99	0.45
1:L:280:TYR:O	1:L:284:VAL:HG23	2.16	0.45
1:A:211:ASP:OD2	1:A:214:ARG:NH1	2.49	0.45
1:C:51:ALA:HA	1:C:63:CYS:SG	2.57	0.45
1:C:171:SER:O	1:C:314:GLN:NE2	2.42	0.45
1:G:385:PHE:O	1:G:388:ARG:HG2	2.16	0.45
1:G:395:LYS:HA	1:G:396:PRO:HD3	1.84	0.45
1:K:49:ARG:NE	1:L:17:GLN:HE22	2.15	0.45
1:K:271:ALA:CB	1:L:6:VAL:HG21	2.45	0.45
1:A:49:ARG:NH2	1:B:368:GLU:OE2	2.49	0.45
1:E:46:PHE:HA	1:E:49:ARG:HG2	1.98	0.45
1:E:133:ARG:HD3	1:F:132:ILE:O	2.16	0.45
1:E:291:LEU:HD21	1:E:386:MET:HE1	1.99	0.45
1:G:303:LEU:HD21	1:G:350:TRP:HH2	1.82	0.45
1:H:1:MET:HG2	1:H:2:GLU:O	2.17	0.45
1:H:32:ASN:OD1	1:H:33:ILE:N	2.50	0.45
1:H:395:LYS:HG3	1:H:396:PRO:O	2.17	0.45
1:J:192:LYS:HD2	1:J:218:GLU:HG3	1.99	0.45
1:K:3:TYR:CE1	1:L:274:LEU:HD22	2.52	0.45
1:L:282:LYS:O	1:L:286:LYS:HG2	2.17	0.45
1:A:296:TYR:HA	1:A:300:PHE:O	2.17	0.45
1:B:50:TYR:HA	1:B:257:ASN:HD22	1.80	0.45
1:B:251:PHE:HD1	1:B:252:PRO:CG	2.29	0.45
1:D:34:THR:O	1:D:39:ARG:NH1	2.50	0.45
1:D:49:ARG:HA	1:D:49:ARG:HD3	1.64	0.45
1:D:343:LEU:HD13	1:D:362:ILE:HD11	1.97	0.45
1:E:252:PRO:HB2	1:F:127:VAL:O	2.16	0.45
1:F:11:ARG:O	1:F:15:ILE:HG13	2.16	0.45
1:F:88:VAL:O	1:F:263:LYS:NZ	2.33	0.45
1:F:214:ARG:HA	1:F:214:ARG:HD3	1.85	0.45
1:G:32:ASN:HD21	1:G:229:PHE:HB3	1.81	0.45
1:G:168:PHE:CD1	1:G:177:HIS:HB3	2.51	0.45
1:H:58:ARG:HH12	1:H:64:LYS:NZ	2.15	0.45
1:I:251:PHE:O	1:I:251:PHE:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:LEU:HD22	1:J:223:SER:O	2.16	0.45
1:A:271:ALA:HA	1:A:274:LEU:HD12	1.98	0.45
1:B:335:MET:HB3	1:B:396:PRO:HG3	1.98	0.45
1:C:197:GLY:O	1:C:201:LEU:N	2.50	0.45
1:E:98:LEU:HD13	1:E:98:LEU:HA	1.85	0.45
1:E:132:ILE:O	1:F:133:ARG:HD3	2.17	0.45
1:F:367:GLN:HG2	1:F:368:GLU:N	2.32	0.45
1:G:125:TRP:HH2	1:G:139:ASN:HB3	1.81	0.45
1:G:411:SER:HB3	1:G:421:ASP:OD1	2.17	0.45
1:K:29:ALA:HB1	1:K:199:HIS:CE1	2.52	0.45
1:K:347:LEU:HD23	1:K:359:PRO:HB3	1.99	0.45
1:L:10:ILE:HG13	1:L:11:ARG:N	2.30	0.45
1:L:242:ASN:O	1:L:245:LYS:HB3	2.16	0.45
1:L:294:ALA:O	1:L:297:GLU:HG2	2.17	0.45
1:B:171:SER:O	1:B:314:GLN:NE2	2.49	0.44
1:C:413:ILE:HG22	1:C:420:GLY:O	2.18	0.44
1:D:388:ARG:NH2	1:I:375:LYS:HD2	2.33	0.44
1:F:90:PRO:HA	1:F:255:VAL:HG21	1.98	0.44
1:G:313:HIS:CE1	1:G:314:GLN:HG3	2.52	0.44
1:A:66:ILE:HD13	1:A:260:LEU:HD13	1.99	0.44
1:D:176:PRO:HB3	1:D:210:GLN:HB3	2.00	0.44
1:E:424:LYS:HA	1:E:424:LYS:HD2	1.86	0.44
1:F:241:GLU:OE1	1:F:241:GLU:N	2.41	0.44
1:D:118:ASP:HA	1:D:349:PRO:HB3	1.98	0.44
1:F:103:ALA:HA	1:F:249:HIS:CG	2.52	0.44
1:G:20:TRP:CH2	1:H:62:GLY:HA2	2.52	0.44
1:G:125:TRP:CE3	1:G:126:LYS:HE3	2.53	0.44
1:L:302:VAL:HB	1:L:309:PHE:CE1	2.53	0.44
1:A:174:PRO:O	1:A:310:THR:HG21	2.18	0.44
1:B:26:LYS:H	1:B:26:LYS:HD2	1.83	0.44
1:B:46:PHE:HB3	1:B:260:LEU:CB	2.47	0.44
1:B:123:SER:HA	1:B:128:SER:OG	2.17	0.44
1:C:298:ARG:HB2	1:C:300:PHE:HD1	1.83	0.44
1:E:18:HIS:NE2	1:F:45:ASP:HB2	2.33	0.44
1:E:111:LEU:O	1:E:138:ILE:HG12	2.18	0.44
1:H:309:PHE:O	1:H:310:THR:HB	2.17	0.44
1:I:228:PHE:HD1	1:I:230:GLY:H	1.65	0.44
1:J:28:ILE:HA	1:J:344:ASN:HD21	1.82	0.44
1:L:58:ARG:HD3	1:L:59:LEU:H	1.81	0.44
1:B:50:TYR:CD1	1:B:257:ASN:HB3	2.52	0.44
1:C:6:VAL:HB	1:D:271:ALA:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LEU:HB3	1:D:364:LEU:HD12	2.00	0.44
1:F:116:VAL:HA	1:F:120:GLY:O	2.18	0.44
1:F:340:ASN:O	1:F:341:ILE:HG13	2.17	0.44
1:G:226:LYS:H	1:G:226:LYS:HG2	1.55	0.44
1:H:102:PHE:O	1:H:133:ARG:NH1	2.50	0.44
1:I:198:ALA:HA	1:I:223:SER:H	1.82	0.44
1:K:158:ILE:O	1:K:189:VAL:HG21	2.18	0.44
1:K:428:PHE:HD2	1:L:40:GLU:HG3	1.83	0.44
1:A:105:THR:O	1:A:133:ARG:NE	2.41	0.44
1:A:256:SER:H	1:B:94:VAL:CG2	2.29	0.44
1:B:22:ARG:NH1	1:B:423:PHE:HB2	2.33	0.44
1:D:106:LYS:HG2	1:D:109:ASP:CG	2.38	0.44
1:D:255:VAL:HG13	1:D:257:ASN:N	2.32	0.44
1:D:292:ALA:HB1	1:D:302:VAL:HG11	1.99	0.44
1:E:101:PHE:CD2	1:E:130:ALA:HB2	2.53	0.44
1:E:378:GLU:O	1:E:382:ILE:HG13	2.17	0.44
1:F:207:LYS:O	1:F:207:LYS:HG3	2.18	0.44
1:F:294:ALA:O	1:F:298:ARG:HG2	2.18	0.44
1:I:318:ASP:OD2	1:I:321:SER:HB2	2.18	0.44
1:J:159:LEU:O	1:J:162:LYS:HG3	2.17	0.44
1:J:421:ASP:HB3	1:J:424:LYS:HG3	2.00	0.44
1:K:115:SER:HB3	1:K:118:ASP:HB2	2.00	0.44
1:B:114:LEU:HD11	1:B:142:PHE:CE1	2.53	0.44
1:B:128:SER:OG	1:B:129:ALA:N	2.50	0.44
1:B:276:PHE:HB3	1:B:415:TYR:HD1	1.82	0.44
1:C:27:LEU:HD13	1:C:364:LEU:HD23	1.99	0.44
1:E:371:ARG:HH22	1:E:416:SER:HB2	1.82	0.44
1:I:62:GLY:HA2	1:J:20:TRP:CZ3	2.53	0.44
1:I:101:PHE:CZ	1:I:167:LEU:HD11	2.52	0.44
1:I:251:PHE:N	1:I:254:VAL:O	2.50	0.44
1:K:76:LEU:HD21	1:K:271:ALA:HB2	1.99	0.44
1:K:130:ALA:HA	1:K:133:ARG:HB3	1.99	0.44
1:L:22:ARG:HB3	1:L:423:PHE:CG	2.53	0.44
1:C:122:ILE:O	1:C:123:SER:OG	2.26	0.44
1:E:255:VAL:CG1	1:E:256:SER:N	2.73	0.44
1:E:271:ALA:HA	1:E:274:LEU:HB2	2.00	0.44
1:I:303:LEU:HD21	1:I:350:TRP:HH2	1.82	0.44
1:J:38:VAL:HG13	1:J:265:GLY:HA3	2.00	0.44
1:J:175:PHE:CE2	1:J:311:GLU:HB2	2.53	0.44
1:C:59:LEU:HB2	1:C:60:TYR:HD1	1.83	0.44
1:C:306:HIS:CD2	1:C:307:LYS:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PRO:HG2	1:D:236:ILE:HG13	2.00	0.44
1:D:225:HIS:HB3	1:D:232:GLN:HA	1.99	0.44
1:E:27:LEU:HD13	1:E:341:ILE:HG23	2.00	0.44
1:E:72:LEU:O	1:E:76:LEU:HB2	2.18	0.44
1:E:115:SER:HA	1:E:125:TRP:NE1	2.33	0.44
1:F:28:ILE:HG22	1:F:344:ASN:HD21	1.83	0.44
1:H:22:ARG:NH2	1:H:411:SER:OG	2.50	0.44
1:L:211:ASP:OD1	1:L:214:ARG:HD2	2.18	0.44
1:L:319:ILE:HD12	1:L:329:ALA:HB1	2.00	0.44
1:A:421:ASP:HB3	1:A:424:LYS:HE3	2.00	0.43
1:A:427:ARG:HB3	1:A:427:ARG:HH11	1.83	0.43
1:B:201:LEU:HB3	1:B:228:PHE:HB2	2.00	0.43
1:B:325:ILE:HG13	1:B:327:PHE:H	1.83	0.43
1:E:8:LYS:HE3	1:E:8:LYS:HB2	1.87	0.43
1:E:212:PRO:HB2	1:E:217:ALA:HB3	1.98	0.43
1:G:82:LYS:HE3	1:G:214:ARG:HH21	1.82	0.43
1:I:133:ARG:HD2	1:I:133:ARG:HA	1.66	0.43
1:J:103:ALA:HA	1:J:249:HIS:CE1	2.53	0.43
1:K:9:PHE:O	1:K:12:ASP:HB3	2.17	0.43
1:L:221:MET:N	1:L:221:MET:HE2	2.33	0.43
1:A:108:GLY:H	1:A:135:LEU:H	1.66	0.43
1:A:238:THR:OG1	1:A:239:THR:N	2.49	0.43
1:C:314:GLN:HA	1:C:364:LEU:O	2.18	0.43
1:D:186:ALA:O	1:D:191:ALA:N	2.41	0.43
1:D:305:GLU:HA	1:D:309:PHE:CE1	2.53	0.43
1:E:66:ILE:HG21	1:E:260:LEU:HD13	2.00	0.43
1:E:112:MET:HG2	1:E:140:HIS:CD2	2.54	0.43
1:F:340:ASN:HB2	1:F:403:VAL:HG21	2.00	0.43
1:F:400:ARG:HE	1:F:404:LYS:NZ	2.13	0.43
1:G:27:LEU:HB2	1:G:343:LEU:HD23	1.99	0.43
1:G:50:TYR:HH	1:H:225:HIS:CD2	2.34	0.43
1:G:50:TYR:OH	1:H:225:HIS:NE2	2.41	0.43
1:J:122:ILE:C	1:J:124:HIS:H	2.21	0.43
1:J:173:PHE:CE2	1:J:209:PHE:HE2	2.36	0.43
1:K:199:HIS:O	1:K:313:HIS:NE2	2.51	0.43
1:K:387:LYS:HE2	1:K:387:LYS:HB3	1.83	0.43
1:D:110:LYS:HG3	1:D:136:LYS:HB3	2.00	0.43
1:G:11:ARG:NH2	1:G:427:ARG:HB3	2.32	0.43
1:H:194:ALA:HB1	1:H:221:MET:HE1	2.00	0.43
1:I:282:LYS:O	1:I:286:LYS:HG2	2.18	0.43
1:I:295:LEU:HD22	1:I:300:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:HIS:CD2	1:L:243:ALA:HA	2.53	0.43
1:A:73:CYS:HB3	1:A:88:VAL:HG11	1.99	0.43
1:C:128:SER:HB2	1:D:252:PRO:HB3	1.99	0.43
1:C:169:GLY:H	1:C:177:HIS:CE1	2.36	0.43
1:C:268:ILE:O	1:C:272:GLU:HG2	2.18	0.43
1:D:198:ALA:HA	1:D:222:GLY:HA2	2.00	0.43
1:D:336:TYR:HD2	1:D:343:LEU:HD21	1.84	0.43
1:E:8:LYS:HA	1:E:11:ARG:HB2	2.00	0.43
1:E:18:HIS:CE1	1:E:425:TYR:HD1	2.35	0.43
1:E:80:LEU:O	1:E:82:LYS:NZ	2.32	0.43
1:E:81:PHE:HB2	1:E:237:LEU:HD22	2.01	0.43
1:E:256:SER:HA	2:F:1430:PLP:O2P	2.19	0.43
1:E:428:PHE:CB	1:F:40:GLU:HB2	2.46	0.43
1:F:249:HIS:C	1:F:253:GLY:HA3	2.38	0.43
1:L:29:ALA:HA	1:L:365:GLY:HA3	2.00	0.43
1:A:92:SER:HB2	1:A:95:VAL:HB	2.00	0.43
1:C:5:ASP:OD1	1:C:5:ASP:N	2.51	0.43
1:C:28:ILE:HB	1:C:31:GLU:HB2	2.00	0.43
1:F:154:MET:HA	1:F:157:LYS:HB2	2.00	0.43
1:G:298:ARG:HB2	1:G:300:PHE:HD1	1.84	0.43
1:G:384:GLU:HA	1:G:387:LYS:HD3	2.01	0.43
1:H:187:GLN:HB3	1:K:126:LYS:HG3	2.01	0.43
1:I:124:HIS:CG	1:I:167:LEU:HD13	2.54	0.43
1:I:395:LYS:HG3	1:I:397:GLU:H	1.84	0.43
1:J:58:ARG:HG2	1:J:59:LEU:H	1.83	0.43
1:K:165:LEU:HD12	1:K:166:ILE:H	1.83	0.43
1:K:175:PHE:CD1	1:K:307:LYS:HD3	2.53	0.43
1:K:368:GLU:O	1:K:372:LEU:HG	2.18	0.43
1:C:290:ALA:HB3	1:C:379:MET:HE3	2.00	0.43
1:C:339:ALA:HB2	1:C:396:PRO:HB3	2.00	0.43
1:C:354:ASN:OD1	1:C:354:ASN:N	2.47	0.43
1:D:312:SER:OG	1:D:313:HIS:N	2.51	0.43
1:E:42:CYS:HA	1:E:261:HIS:HB2	2.00	0.43
1:E:343:LEU:HD23	1:E:364:LEU:HD11	2.00	0.43
1:F:54:LEU:HB3	1:F:55:PRO:HD2	2.00	0.43
1:F:366:THR:O	1:F:366:THR:OG1	2.36	0.43
1:I:72:LEU:HD21	1:J:6:VAL:HG13	1.99	0.43
1:J:112:MET:O	1:J:167:LEU:HB2	2.17	0.43
1:J:306:HIS:CD2	1:J:307:LYS:HG2	2.53	0.43
1:J:325:ILE:HG23	1:J:390:ALA:HB1	2.01	0.43
1:K:6:VAL:N	1:K:7:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:272:GLU:OE1	1:K:371:ARG:NH2	2.51	0.43
1:A:105:THR:HA	1:A:164:LYS:HZ1	1.84	0.43
1:B:287:ASN:HA	1:B:379:MET:HE1	2.01	0.43
1:C:90:PRO:HG3	1:C:250:VAL:HG21	2.00	0.43
1:C:348:LEU:N	1:C:351:ASP:OD2	2.40	0.43
1:E:289:LYS:HB3	1:E:310:THR:HG23	1.95	0.43
1:F:28:ILE:HG13	1:F:31:GLU:HB3	2.01	0.43
1:G:114:LEU:O	1:G:125:TRP:NE1	2.38	0.43
1:G:375:LYS:NZ	1:G:415:TYR:OH	2.51	0.43
1:H:119:GLY:HA3	1:H:172:LEU:HB2	2.00	0.43
1:J:154:MET:HG3	1:J:155:VAL:N	2.33	0.43
1:J:368:GLU:O	1:J:372:LEU:HG	2.19	0.43
1:K:398:LYS:HE2	1:K:398:LYS:HB3	1.82	0.43
1:L:371:ARG:NH2	1:L:416:SER:HB2	2.34	0.43
1:A:50:TYR:CZ	1:A:257:ASN:HB3	2.52	0.43
1:A:122:ILE:O	1:A:123:SER:OG	2.29	0.43
1:B:394:GLU:HG2	1:B:395:LYS:H	1.84	0.43
1:D:307:LYS:O	1:D:308:ASP:HB2	2.19	0.43
1:D:404:LYS:O	1:D:408:LYS:HB2	2.19	0.43
1:E:78:LYS:HE2	1:E:85:HIS:HA	1.99	0.43
1:G:82:LYS:HB2	1:G:214:ARG:NH2	2.33	0.43
1:G:155:VAL:O	1:G:159:LEU:HB2	2.19	0.43
1:G:246:ILE:O	1:G:250:VAL:HG23	2.19	0.43
1:I:141:PRO:HG2	1:I:154:MET:HA	2.00	0.43
1:I:294:ALA:HB2	1:I:380:GLU:HG2	2.00	0.43
1:J:97:ASN:HB3	1:J:101:PHE:HE2	1.83	0.43
1:L:238:THR:OG1	1:L:239:THR:N	2.51	0.43
1:A:326:GLU:HG2	1:D:157:LYS:HA	1.99	0.43
1:C:419:GLU:O	1:K:398:LYS:NZ	2.52	0.43
1:E:112:MET:HB2	1:E:112:MET:HE3	1.83	0.43
1:H:399:VAL:O	1:H:403:VAL:HG23	2.19	0.43
1:I:185:ALA:O	1:I:189:VAL:HG23	2.19	0.43
1:J:212:PRO:HG2	1:J:220:LEU:HD12	2.01	0.43
1:L:19:GLU:HA	1:L:22:ARG:NE	2.32	0.43
1:B:325:ILE:HG23	1:B:326:GLU:N	2.31	0.43
1:E:34:THR:HG22	1:F:48:HIS:NE2	2.34	0.43
1:E:429:TYR:CD1	1:F:37:ALA:HA	2.54	0.43
1:H:116:VAL:HG21	1:H:122:ILE:HG23	2.01	0.43
1:J:291:LEU:HB2	1:J:379:MET:HB3	1.99	0.43
1:J:399:VAL:O	1:J:403:VAL:HG13	2.18	0.43
1:L:199:HIS:O	1:L:313:HIS:NE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:O	1:A:218:GLU:N	2.46	0.42
1:B:268:ILE:O	1:B:272:GLU:HG3	2.19	0.42
1:C:6:VAL:HG21	1:D:76:LEU:HD21	2.01	0.42
1:C:186:ALA:O	1:C:191:ALA:N	2.38	0.42
1:C:242:ASN:O	1:C:246:ILE:HG22	2.19	0.42
1:D:254:VAL:HG13	1:D:255:VAL:H	1.84	0.42
1:E:256:SER:HB3	1:F:92:SER:HB2	2.01	0.42
1:E:336:TYR:HB3	1:E:343:LEU:HD11	2.01	0.42
1:F:386:MET:HA	1:F:389:ILE:HD11	2.01	0.42
1:I:169:GLY:HA3	1:I:196:ASP:O	2.19	0.42
1:K:109:ASP:OD1	1:K:110:LYS:N	2.47	0.42
1:K:147:MET:HB2	1:K:174:PRO:HG2	2.01	0.42
1:A:226:LYS:HB3	1:A:227:THR:H	1.51	0.42
1:A:348:LEU:HG	1:A:361:GLY:HA3	2.01	0.42
1:C:225:HIS:CD2	1:C:225:HIS:H	2.36	0.42
1:D:251:PHE:HA	1:D:252:PRO:HA	1.84	0.42
1:D:330:SER:HB2	1:D:357:ASP:O	2.18	0.42
1:D:395:LYS:HA	1:D:396:PRO:HD3	1.85	0.42
1:E:22:ARG:HA	1:E:423:PHE:CE1	2.54	0.42
1:E:49:ARG:HA	1:F:31:GLU:HG3	2.00	0.42
1:G:158:ILE:HG13	1:G:166:ILE:HG12	2.01	0.42
1:H:111:LEU:HB3	1:H:137:VAL:HG13	2.01	0.42
1:H:122:ILE:H	1:H:122:ILE:HG12	1.63	0.42
1:H:283:GLN:HA	1:H:286:LYS:HB2	2.02	0.42
1:K:412:THR:HA	1:K:420:GLY:O	2.20	0.42
1:B:75:GLU:HA	1:B:78:LYS:HB2	2.01	0.42
1:C:394:GLU:OE1	1:C:395:LYS:N	2.33	0.42
1:E:144:PRO:C	1:E:146:GLU:H	2.23	0.42
1:H:105:THR:O	1:H:133:ARG:NH1	2.53	0.42
1:H:202:GLY:H	1:H:227:THR:HB	1.84	0.42
1:L:14:SER:O	1:L:17:GLN:HB3	2.19	0.42
1:A:27:LEU:HD13	1:A:364:LEU:HD22	2.01	0.42
1:A:72:LEU:HD22	1:A:72:LEU:HA	1.84	0.42
1:C:58:ARG:NH2	1:C:66:ILE:HG22	2.34	0.42
1:C:374:MET:SD	1:C:378:GLU:HG2	2.60	0.42
1:D:147:MET:HB2	1:D:174:PRO:HG3	2.01	0.42
1:E:39:ARG:HE	1:F:48:HIS:CE1	2.37	0.42
1:F:58:ARG:NH2	1:F:70:GLU:OE1	2.48	0.42
1:G:383:ALA:O	1:G:387:LYS:HB3	2.19	0.42
1:I:336:TYR:CD2	1:I:343:LEU:HD21	2.54	0.42
1:J:198:ALA:O	1:J:226:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:ARG:HB2	1:L:132:ILE:HG23	2.01	0.42
1:K:224:THR:HG21	1:K:266:LEU:HD13	2.00	0.42
1:K:395:LYS:HB3	1:K:398:LYS:HE2	2.01	0.42
1:L:175:PHE:CZ	1:L:307:LYS:HB3	2.53	0.42
1:A:211:ASP:HA	1:A:212:PRO:HD2	1.88	0.42
1:E:129:ALA:C	1:E:131:GLY:H	2.22	0.42
1:F:29:ALA:HA	1:F:367:GLN:HE22	1.85	0.42
1:F:42:CYS:HA	1:F:261:HIS:HB2	2.02	0.42
1:G:298:ARG:HB3	1:G:387:LYS:HB2	2.02	0.42
1:H:152:ASP:HB3	1:L:245:LYS:HD2	2.01	0.42
1:I:84:GLU:CD	1:I:240:LYS:H	2.23	0.42
1:J:11:ARG:HG3	1:J:425:TYR:OH	2.19	0.42
1:J:219:TYR:OH	1:J:242:ASN:HB3	2.20	0.42
1:K:36:LEU:HD12	1:K:420:GLY:HA3	2.01	0.42
1:L:175:PHE:CZ	1:L:307:LYS:HD3	2.53	0.42
1:L:236:ILE:HG21	1:L:246:ILE:HG12	2.00	0.42
1:A:46:PHE:HB3	1:A:260:LEU:CB	2.48	0.42
1:C:283:GLN:NE2	1:C:287:ASN:OD1	2.42	0.42
1:C:369:CYS:HB3	1:C:374:MET:HE2	2.00	0.42
1:D:111:LEU:HD11	1:D:167:LEU:HB2	2.02	0.42
1:D:163:PRO:O	1:D:191:ALA:HB2	2.20	0.42
1:E:252:PRO:HA	1:E:255:VAL:HG22	2.02	0.42
1:E:405:GLU:O	1:E:409:GLU:HG2	2.19	0.42
1:H:366:THR:O	1:H:370:THR:OG1	2.31	0.42
1:I:18:HIS:CD2	1:J:45:ASP:HB2	2.54	0.42
1:K:55:PRO:O	1:K:57:LYS:NZ	2.52	0.42
1:K:271:ALA:HA	1:K:274:LEU:HB2	2.02	0.42
1:K:323:PRO:C	1:K:325:ILE:H	2.23	0.42
1:A:281:ALA:O	1:A:285:ILE:HG13	2.20	0.42
1:B:70:GLU:O	1:B:74:ILE:HG12	2.19	0.42
1:B:250:VAL:O	1:B:255:VAL:CB	2.61	0.42
1:C:123:SER:HA	1:C:128:SER:HB3	2.02	0.42
1:D:154:MET:O	1:D:158:ILE:HG13	2.19	0.42
1:D:238:THR:OG1	1:D:239:THR:N	2.49	0.42
1:D:307:LYS:HE3	1:D:307:LYS:HB3	1.69	0.42
1:J:92:SER:H	1:J:233:GLY:CA	2.32	0.42
1:J:130:ALA:HB1	1:J:134:GLY:HA3	2.02	0.42
1:K:132:ILE:HG21	1:L:98:LEU:HD11	2.02	0.42
1:K:245:LYS:O	1:K:249:HIS:HD2	2.03	0.42
1:E:244:ASP:O	1:E:248:SER:N	2.53	0.42
1:E:344:ASN:ND2	1:F:60:TYR:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:LEU:HA	1:F:54:LEU:HD23	1.50	0.42
1:F:87:ASN:OD1	1:F:90:PRO:HD3	2.20	0.42
1:G:53:GLY:HA3	1:G:89:GLN:CD	2.39	0.42
1:H:171:SER:HB2	1:H:363:ARG:NH2	2.34	0.42
1:A:50:TYR:CE2	1:B:30:SER:HB3	2.54	0.42
1:A:115:SER:OG	1:A:117:PRO:HD2	2.19	0.42
1:A:263:LYS:HD3	1:A:263:LYS:HA	1.78	0.42
1:A:316:ILE:HA	1:A:362:ILE:O	2.20	0.42
1:B:236:ILE:HD12	1:B:246:ILE:HD11	2.01	0.42
1:E:195:TYR:HE2	1:E:210:GLN:HE21	1.66	0.42
1:G:257:ASN:C	1:G:259:HIS:H	2.22	0.42
1:H:107:PRO:O	1:I:188:GLU:HG3	2.19	0.42
1:H:218:GLU:OE2	1:H:242:ASN:ND2	2.40	0.42
1:H:322:SER:HA	1:H:323:PRO:HD3	1.77	0.42
1:I:55:PRO:HA	1:I:58:ARG:HE	1.85	0.42
1:I:110:LYS:HA	1:I:136:LYS:O	2.20	0.42
1:J:80:LEU:HD21	1:J:205:ALA:HB1	2.01	0.42
1:J:245:LYS:O	1:J:249:HIS:HD2	2.02	0.42
1:K:22:ARG:CZ	1:K:411:SER:HB3	2.49	0.42
1:K:63:CYS:HA	1:K:66:ILE:HD12	2.02	0.42
1:K:84:GLU:OE1	1:K:240:LYS:HE3	2.20	0.42
1:K:425:TYR:OH	1:L:40:GLU:OE1	2.33	0.42
1:L:389:ILE:HD11	1:L:399:VAL:HG11	2.02	0.42
1:C:330:SER:O	1:C:334:LYS:HB2	2.20	0.42
1:D:186:ALA:HA	1:D:189:VAL:HG12	2.01	0.42
1:E:381:GLU:HG2	1:E:406:PHE:CE1	2.54	0.42
1:G:125:TRP:HE3	1:G:126:LYS:HE3	1.85	0.42
1:I:320:GLU:HG3	1:I:321:SER:N	2.34	0.42
1:J:110:LYS:HE3	1:J:110:LYS:HB2	1.84	0.42
1:K:115:SER:HA	1:K:125:TRP:CZ2	2.54	0.42
1:L:39:ARG:NH1	1:L:424:LYS:O	2.53	0.42
1:L:154:MET:O	1:L:158:ILE:HG13	2.20	0.42
1:B:149:ILE:O	1:B:178:PRO:HG3	2.19	0.41
1:B:251:PHE:CD1	1:B:252:PRO:N	2.88	0.41
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.83	0.41
1:B:348:LEU:H	1:B:351:ASP:CB	2.30	0.41
1:C:388:ARG:O	1:C:394:GLU:N	2.53	0.41
1:D:171:SER:HA	1:D:199:HIS:HD2	1.85	0.41
1:G:348:LEU:H	1:G:351:ASP:HB2	1.85	0.41
1:I:345:LYS:HA	1:I:362:ILE:HG22	2.02	0.41
1:J:289:LYS:NZ	1:J:308:ASP:OD1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:HIS:NE2	1:K:154:MET:SD	2.94	0.41
1:K:337:GLU:HA	1:K:342:ILE:HG13	2.02	0.41
1:A:294:ALA:HB2	1:A:380:GLU:HG2	2.03	0.41
1:B:14:SER:O	1:B:17:GLN:HB3	2.20	0.41
1:C:64:LYS:HE3	1:C:65:TYR:CE2	2.55	0.41
1:D:107:PRO:HG3	1:D:133:ARG:NH1	2.34	0.41
1:D:348:LEU:HD13	1:D:360:SER:HB2	2.01	0.41
1:D:376:GLU:O	1:D:380:GLU:N	2.52	0.41
1:D:429:TYR:OXT	1:D:429:TYR:CD2	2.73	0.41
1:F:53:GLY:HA2	1:F:251:PHE:CD1	2.55	0.41
1:G:34:THR:HG22	1:G:229:PHE:O	2.19	0.41
1:H:227:THR:HB	1:H:228:PHE:H	1.48	0.41
1:J:77:SER:HB2	1:J:237:LEU:HD21	2.02	0.41
1:K:111:LEU:HD23	1:K:124:HIS:HB3	2.02	0.41
1:L:174:PRO:HB2	1:L:175:PHE:HD1	1.85	0.41
1:A:72:LEU:HG	1:B:9:PHE:CE2	2.54	0.41
1:B:8:LYS:HB2	1:B:8:LYS:HE3	1.74	0.41
1:C:126:LYS:HA	1:C:131:GLY:HA3	2.02	0.41
1:C:232:GLN:NE2	1:D:257:ASN:OD1	2.53	0.41
1:E:15:ILE:HG12	1:E:425:TYR:CG	2.55	0.41
1:E:20:TRP:O	1:E:23:GLU:HG2	2.21	0.41
1:E:298:ARG:HG3	1:E:387:LYS:HD2	2.02	0.41
1:G:11:ARG:CZ	1:G:427:ARG:HD2	2.50	0.41
1:I:27:LEU:HD12	1:I:364:LEU:HB3	2.01	0.41
1:J:121:HIS:HB2	1:J:171:SER:H	1.85	0.41
1:K:226:LYS:C	1:K:228:PHE:H	2.23	0.41
1:A:114:LEU:HD12	1:A:118:ASP:O	2.20	0.41
1:A:192:LYS:NZ	1:A:218:GLU:OE2	2.42	0.41
1:A:274:LEU:HD13	1:B:3:TYR:HE1	1.85	0.41
1:A:388:ARG:O	1:A:393:LYS:N	2.54	0.41
1:B:129:ALA:O	1:B:130:ALA:HB3	2.20	0.41
1:B:146:GLU:HA	1:B:304:CYS:SG	2.60	0.41
1:B:426:LEU:HD12	1:B:426:LEU:HA	1.89	0.41
1:C:33:ILE:HG13	1:D:48:HIS:CE1	2.55	0.41
1:E:17:GLN:HE21	1:E:17:GLN:HB2	1.64	0.41
1:F:23:GLU:O	1:F:340:ASN:OD1	2.38	0.41
1:F:226:LYS:HD3	1:F:226:LYS:HA	1.93	0.41
1:I:413:ILE:N	1:I:420:GLY:O	2.52	0.41
1:J:51:ALA:HB3	1:J:258:HIS:NE2	2.35	0.41
1:A:40:GLU:HB2	1:B:428:PHE:HB2	2.02	0.41
1:A:317:ILE:HB	1:A:362:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:HB3	1:B:142:PHE:CE1	2.55	0.41
1:B:251:PHE:HD1	1:B:252:PRO:HG3	1.85	0.41
1:E:95:VAL:O	1:E:254:VAL:HG11	2.21	0.41
1:E:111:LEU:O	1:E:138:ILE:N	2.49	0.41
1:E:388:ARG:HH21	1:E:399:VAL:HG22	1.85	0.41
1:E:428:PHE:CG	1:F:40:GLU:HB2	2.56	0.41
1:G:103:ALA:HA	1:G:249:HIS:ND1	2.35	0.41
1:H:180:ALA:HB3	1:L:106:LYS:NZ	2.34	0.41
1:A:34:THR:HG22	1:A:229:PHE:O	2.21	0.41
1:B:26:LYS:HD3	1:B:368:GLU:CG	2.50	0.41
1:C:90:PRO:HG2	1:C:236:ILE:HG13	2.01	0.41
1:D:110:LYS:HD2	1:D:138:ILE:HD11	2.03	0.41
1:E:256:SER:HA	2:F:1430:PLP:O1P	2.19	0.41
1:G:65:TYR:O	1:G:68:GLU:HB2	2.20	0.41
1:H:117:PRO:HB3	1:H:354:ASN:OD1	2.20	0.41
1:I:38:VAL:HG11	1:I:231:PRO:HD3	2.03	0.41
1:J:130:ALA:O	1:J:134:GLY:N	2.53	0.41
1:A:204:ILE:HD12	1:A:210:GLN:O	2.20	0.41
1:B:92:SER:HB3	1:B:95:VAL:HG23	2.02	0.41
1:B:148:ASN:OD1	1:B:178:PRO:HD3	2.21	0.41
1:B:154:MET:SD	1:B:182:ALA:HB2	2.59	0.41
1:D:173:PHE:HZ	1:D:177:HIS:CE1	2.39	0.41
1:G:52:GLU:HG3	1:G:59:LEU:HD13	2.01	0.41
1:G:149:ILE:HD11	1:G:154:MET:SD	2.60	0.41
1:G:352:ASP:OD1	1:G:352:ASP:N	2.52	0.41
1:H:211:ASP:O	1:H:215:GLU:HB2	2.20	0.41
1:I:208:GLN:HG3	1:I:209:PHE:H	1.85	0.41
1:I:300:PHE:CD1	1:I:325:ILE:HD11	2.56	0.41
1:K:119:GLY:HA2	1:K:172:LEU:HB2	2.01	0.41
1:L:322:SER:HB3	1:L:325:ILE:HG12	2.02	0.41
1:A:337:GLU:HG3	1:B:61:GLN:HB3	2.02	0.41
1:B:174:PRO:HB3	1:B:316:ILE:HD11	2.02	0.41
1:C:59:LEU:O	1:C:60:TYR:HB2	2.19	0.41
1:C:225:HIS:HE1	1:D:50:TYR:HE2	1.69	0.41
1:D:34:THR:HG23	1:D:39:ARG:CG	2.48	0.41
1:E:282:LYS:O	1:E:286:LYS:HD3	2.21	0.41
1:F:35:SER:O	1:F:39:ARG:HG3	2.20	0.41
1:G:10:ILE:H	1:G:10:ILE:HG12	1.54	0.41
1:G:64:LYS:O	1:G:68:GLU:HG3	2.20	0.41
1:H:101:PHE:CE1	1:H:167:LEU:HD11	2.56	0.41
1:H:228:PHE:HA	1:H:273:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:302:VAL:HG22	1:H:317:ILE:HG22	2.02	0.41
1:H:339:ALA:HB2	1:H:396:PRO:HB3	2.03	0.41
1:H:388:ARG:HB3	1:H:394:GLU:OE1	2.20	0.41
1:I:47:MET:HG2	1:I:261:HIS:HB3	2.03	0.41
1:I:107:PRO:HD3	1:I:133:ARG:NH2	2.36	0.41
1:J:175:PHE:CD2	1:J:176:PRO:HD2	2.56	0.41
1:J:329:ALA:O	1:J:362:ILE:HD11	2.20	0.41
1:K:168:PHE:CD2	1:K:179:VAL:HG12	2.55	0.41
1:A:5:ASP:N	1:A:5:ASP:OD1	2.54	0.41
1:A:229:PHE:CZ	1:A:273:MET:HE2	2.56	0.41
1:B:21:MET:O	1:B:26:LYS:NZ	2.45	0.41
1:B:30:SER:HA	1:B:226:LYS:HD2	2.02	0.41
1:B:125:TRP:O	1:B:128:SER:HB3	2.21	0.41
1:B:228:PHE:HA	1:B:273:MET:HE3	2.02	0.41
1:B:280:TYR:HA	1:B:415:TYR:CZ	2.56	0.41
1:B:319:ILE:HD12	1:B:319:ILE:HA	1.99	0.41
1:B:389:ILE:HD11	1:B:399:VAL:HG21	2.03	0.41
1:C:18:HIS:HE1	1:C:39:ARG:NH2	2.19	0.41
1:C:28:ILE:HG22	1:C:30:SER:H	1.85	0.41
1:D:66:ILE:HG21	1:D:260:LEU:HD13	2.02	0.41
1:D:300:PHE:HE1	1:D:387:LYS:HA	1.85	0.41
1:D:367:GLN:CD	1:D:367:GLN:H	2.23	0.41
1:D:371:ARG:NH1	1:D:413:ILE:HG12	2.35	0.41
1:E:105:THR:OG1	1:E:133:ARG:NH1	2.54	0.41
1:E:155:VAL:O	1:E:159:LEU:HG	2.21	0.41
1:E:198:ALA:HB3	2:E:1430:PLP:C2	2.50	0.41
1:F:54:LEU:O	1:F:58:ARG:NH2	2.53	0.41
1:G:201:LEU:O	1:G:204:ILE:HB	2.21	0.41
1:H:112:MET:HB3	1:H:166:ILE:HA	2.02	0.41
1:H:150:ASP:HB2	1:H:153:ALA:HB3	2.03	0.41
1:H:424:LYS:HE3	1:H:426:LEU:HD11	2.02	0.41
1:I:48:HIS:HD2	1:J:34:THR:H	1.66	0.41
1:I:168:PHE:CE2	1:I:179:VAL:HA	2.55	0.41
1:J:57:LYS:HE3	1:J:57:LYS:HB3	1.87	0.41
1:J:110:LYS:HB2	1:J:163:PRO:HA	2.03	0.41
1:K:319:ILE:HD13	1:K:362:ILE:HG13	2.03	0.41
1:K:336:TYR:CD1	1:K:389:ILE:HD12	2.56	0.41
1:L:123:SER:O	1:L:130:ALA:HB2	2.20	0.41
1:L:168:PHE:CE2	1:L:179:VAL:HA	2.56	0.41
1:A:274:LEU:HD13	1:B:3:TYR:CE1	2.56	0.41
1:A:295:LEU:HG	1:A:300:PHE:CD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLU:HG3	1:C:306:HIS:HE1	1.86	0.41
1:D:84:GLU:HB3	1:D:240:LYS:HG2	2.03	0.41
1:E:72:LEU:HD22	1:E:76:LEU:HD22	2.03	0.41
1:F:369:CYS:HB3	1:F:374:MET:HG3	2.01	0.41
1:G:40:GLU:HB2	1:H:428:PHE:HB2	2.03	0.41
1:G:214:ARG:H	1:G:214:ARG:HG2	1.49	0.41
1:G:227:THR:HG23	1:G:228:PHE:N	2.32	0.41
1:G:330:SER:HA	1:G:345:LYS:HD3	2.03	0.41
1:H:113:ALA:O	1:H:139:ASN:HA	2.21	0.41
1:H:150:ASP:O	1:H:154:MET:HB2	2.21	0.41
1:H:193:ILE:O	1:H:218:GLU:N	2.54	0.41
1:H:286:LYS:HB3	1:H:376:GLU:OE2	2.21	0.41
1:I:347:LEU:HD12	1:I:359:PRO:HB3	2.02	0.41
1:J:115:SER:OG	1:J:118:ASP:HB2	2.21	0.41
1:L:25:ILE:HG13	1:L:341:ILE:HG23	2.03	0.41
1:L:115:SER:OG	1:L:117:PRO:HD2	2.20	0.41
1:L:336:TYR:HB3	1:L:341:ILE:HB	2.02	0.41
1:A:28:ILE:H	1:A:28:ILE:HG12	1.63	0.40
1:A:110:LYS:HE2	1:A:110:LYS:HB2	1.80	0.40
1:A:135:LEU:HD11	1:C:190:GLY:HA2	2.03	0.40
1:C:229:PHE:CD2	1:C:371:ARG:HD3	2.55	0.40
1:E:60:TYR:HD1	1:E:60:TYR:HA	1.67	0.40
1:E:174:PRO:HA	1:E:312:SER:HB3	2.02	0.40
1:F:103:ALA:HA	1:F:249:HIS:CD2	2.56	0.40
1:F:381:GLU:O	1:F:384:GLU:HB3	2.20	0.40
1:J:214:ARG:N	1:J:214:ARG:HD2	2.37	0.40
1:L:30:SER:OG	1:L:363:ARG:NH2	2.54	0.40
1:L:87:ASN:ND2	1:L:247:ASP:OD1	2.54	0.40
1:A:87:ASN:HB3	1:A:236:ILE:HB	2.04	0.40
1:A:108:GLY:H	1:A:134:GLY:HA2	1.85	0.40
1:A:110:LYS:HE3	1:A:161:GLU:O	2.21	0.40
1:A:129:ALA:HA	1:A:132:ILE:HG13	2.03	0.40
1:A:131:GLY:O	1:B:133:ARG:NH1	2.53	0.40
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.91	0.40
1:D:110:LYS:NZ	1:D:161:GLU:HB3	2.36	0.40
1:E:6:VAL:O	1:E:10:ILE:HG13	2.21	0.40
1:G:116:VAL:HG22	1:G:125:TRP:CD1	2.57	0.40
1:H:70:GLU:O	1:H:74:ILE:HG13	2.21	0.40
1:H:81:PHE:CZ	1:H:205:ALA:HB2	2.56	0.40
1:H:123:SER:N	1:H:128:SER:OG	2.54	0.40
1:H:143:ASP:HA	1:H:144:PRO:HD3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:SER:HB3	1:H:325:ILE:HD13	2.04	0.40
1:J:385:PHE:HD1	1:J:388:ARG:HD2	1.84	0.40
1:K:418:ASP:N	1:K:418:ASP:OD1	2.54	0.40
1:L:46:PHE:HB3	1:L:260:LEU:HB3	2.03	0.40
1:L:395:LYS:HA	1:L:396:PRO:HD3	1.82	0.40
1:A:184:GLU:O	1:A:188:GLU:HG3	2.22	0.40
1:A:291:LEU:HB2	1:A:379:MET:HB3	2.03	0.40
1:B:240:LYS:HB2	1:B:240:LYS:HE3	1.85	0.40
1:C:102:PHE:HA	1:C:133:ARG:HG2	2.03	0.40
1:C:297:GLU:HG3	1:C:298:ARG:NH1	2.37	0.40
1:F:37:ALA:HB1	1:F:268:ILE:HD13	2.02	0.40
1:F:204:ILE:HG23	1:F:212:PRO:HD2	2.02	0.40
1:G:91:THR:O	1:G:233:GLY:HA2	2.22	0.40
1:H:103:ALA:HA	1:H:249:HIS:CD2	2.56	0.40
1:L:100:VAL:HG11	1:L:221:MET:HE1	2.03	0.40
1:L:295:LEU:O	1:L:300:PHE:HB2	2.21	0.40
1:B:184:GLU:H	1:B:184:GLU:HG2	1.71	0.40
1:B:305:GLU:OE1	1:B:305:GLU:N	2.52	0.40
1:C:87:ASN:OD1	1:C:90:PRO:HD3	2.21	0.40
1:D:353:VAL:HG13	1:D:354:ASN:N	2.36	0.40
1:E:356:SER:HB3	1:E:358:ASN:H	1.84	0.40
1:F:125:TRP:O	1:F:130:ALA:HB3	2.21	0.40
1:G:54:LEU:HD12	1:G:55:PRO:CD	2.51	0.40
1:H:24:SER:HA	1:H:340:ASN:HB3	2.03	0.40
1:H:91:THR:O	1:H:233:GLY:HA2	2.21	0.40
1:H:91:THR:C	1:H:233:GLY:HA2	2.41	0.40
1:H:258:HIS:O	1:H:263:LYS:NZ	2.48	0.40
1:I:328:SER:OG	1:I:358:ASN:OD1	2.38	0.40
1:J:14:SER:O	1:J:18:HIS:HD2	2.04	0.40
1:J:108:GLY:N	1:J:135:LEU:HD12	2.36	0.40
1:J:395:LYS:HA	1:J:396:PRO:HD3	1.94	0.40
1:K:21:MET:O	1:K:26:LYS:NZ	2.31	0.40
1:K:114:LEU:HD23	1:K:140:HIS:HB3	2.03	0.40
1:K:135:LEU:HD23	1:K:136:LYS:HE2	2.03	0.40
1:L:225:HIS:CE1	1:L:233:GLY:H	2.40	0.40
1:L:303:LEU:HB2	1:L:316:ILE:O	2.22	0.40
1:A:427:ARG:NH1	1:A:429:TYR:OXT	2.50	0.40
1:D:157:LYS:HG3	1:D:161:GLU:HG3	2.04	0.40
1:E:149:ILE:HD12	1:E:168:PHE:HE1	1.85	0.40
1:E:305:GLU:HA	1:E:309:PHE:CE1	2.57	0.40
1:F:126:LYS:C	1:F:128:SER:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:GLN:HE21	1:H:258:HIS:CE1	2.40	0.40
1:I:51:ALA:O	1:I:58:ARG:HD2	2.22	0.40
1:I:55:PRO:HB3	1:I:67:ASP:HB3	2.03	0.40
1:I:105:THR:HG23	1:I:109:ASP:CB	2.50	0.40
1:I:169:GLY:H	1:I:177:HIS:HD2	1.68	0.40
1:I:413:ILE:HG22	1:I:420:GLY:O	2.21	0.40
1:J:45:ASP:O	1:J:48:HIS:ND1	2.49	0.40
1:J:175:PHE:CZ	1:J:307:LYS:HB3	2.57	0.40
1:J:321:SER:O	1:J:322:SER:OG	2.32	0.40
1:J:336:TYR:CD2	1:J:343:LEU:HD21	2.56	0.40
1:J:398:LYS:HA	1:J:398:LYS:HD2	1.86	0.40
1:L:284:VAL:HG22	1:L:370:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/429 (98%)	391 (93%)	28 (7%)	3 (1%)	22	60
1	B	418/429 (97%)	382 (91%)	32 (8%)	4 (1%)	15	53
1	C	414/429 (96%)	375 (91%)	38 (9%)	1 (0%)	47	82
1	D	421/429 (98%)	375 (89%)	44 (10%)	2 (0%)	29	68
1	E	425/429 (99%)	380 (89%)	43 (10%)	2 (0%)	29	68
1	F	412/429 (96%)	368 (89%)	38 (9%)	6 (2%)	10	42
1	G	427/429 (100%)	394 (92%)	33 (8%)	0	100	100
1	H	423/429 (99%)	378 (89%)	44 (10%)	1 (0%)	47	82
1	I	425/429 (99%)	398 (94%)	26 (6%)	1 (0%)	47	82
1	J	427/429 (100%)	383 (90%)	41 (10%)	3 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	416/429 (97%)	377 (91%)	38 (9%)	1 (0%)	47	82
1	L	410/429 (96%)	368 (90%)	40 (10%)	2 (0%)	29	68
All	All	5040/5148 (98%)	4569 (91%)	445 (9%)	26 (0%)	29	68

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	B	127	VAL
1	C	127	VAL
1	F	54	LEU
1	F	127	VAL
1	H	127	VAL
1	I	127	VAL
1	J	127	VAL
1	A	226	LYS
1	B	251	PHE
1	E	255	VAL
1	F	252	PRO
1	L	55	PRO
1	A	256	SER
1	B	351	ASP
1	D	255	VAL
1	E	243	ALA
1	F	226	LYS
1	D	133	ARG
1	F	162	LYS
1	B	253	GLY
1	J	353	VAL
1	J	254	VAL
1	L	251	PHE
1	F	254	VAL
1	K	127	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/359 (99%)	332 (93%)	25 (7%)	15	47
1	B	355/359 (99%)	334 (94%)	21 (6%)	19	54
1	C	350/359 (98%)	327 (93%)	23 (7%)	16	49
1	D	356/359 (99%)	325 (91%)	31 (9%)	10	37
1	E	357/359 (99%)	327 (92%)	30 (8%)	11	38
1	F	348/359 (97%)	320 (92%)	28 (8%)	12	40
1	G	359/359 (100%)	327 (91%)	32 (9%)	9	35
1	H	357/359 (99%)	328 (92%)	29 (8%)	11	40
1	I	357/359 (99%)	334 (94%)	23 (6%)	17	51
1	J	359/359 (100%)	334 (93%)	25 (7%)	15	47
1	K	352/359 (98%)	323 (92%)	29 (8%)	11	39
1	L	350/359 (98%)	309 (88%)	41 (12%)	5	22
All	All	4257/4308 (99%)	3920 (92%)	337 (8%)	12	41

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	28	ILE
1	A	50	TYR
1	A	72	LEU
1	A	95	VAL
1	A	98	LEU
1	A	122	ILE
1	A	137	VAL
1	A	152	ASP
1	A	156	LYS
1	A	181	ASP
1	A	209	PHE
1	A	226	LYS
1	A	229	PHE
1	A	258	HIS
1	A	310	THR
1	A	311	GLU
1	A	326	GLU
1	A	344	ASN
1	A	346	ASN
1	A	352	ASP
1	A	395	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	410	TYR
1	A	414	HIS
1	A	427	ARG
1	B	5	ASP
1	B	26	LYS
1	B	50	TYR
1	B	54	LEU
1	B	102	PHE
1	B	127	VAL
1	B	138	ILE
1	B	143	ASP
1	B	173	PHE
1	B	229	PHE
1	B	237	LEU
1	B	256	SER
1	B	258	HIS
1	B	262	HIS
1	B	303	LEU
1	B	316	ILE
1	B	322	SER
1	B	355	ASN
1	B	376	GLU
1	B	381	GLU
1	B	392	ASP
1	C	5	ASP
1	C	8	LYS
1	C	21	MET
1	C	26	LYS
1	C	57	LYS
1	C	59	LEU
1	C	105	THR
1	C	116	VAL
1	C	126	LYS
1	C	127	VAL
1	C	139	ASN
1	C	184	GLU
1	C	189	VAL
1	C	214	ARG
1	C	263	LYS
1	C	268	ILE
1	C	313	HIS
1	C	382	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	386	MET
1	C	394	GLU
1	C	397	GLU
1	C	412	THR
1	C	413	ILE
1	D	5	ASP
1	D	26	LYS
1	D	49	ARG
1	D	50	TYR
1	D	52	GLU
1	D	60	TYR
1	D	98	LEU
1	D	135	LEU
1	D	159	LEU
1	D	160	GLU
1	D	173	PHE
1	D	177	HIS
1	D	188	GLU
1	D	189	VAL
1	D	199	HIS
1	D	214	ARG
1	D	226	LYS
1	D	241	GLU
1	D	257	ASN
1	D	285	ILE
1	D	307	LYS
1	D	324	ASP
1	D	325	ILE
1	D	343	LEU
1	D	350	TRP
1	D	352	ASP
1	D	354	ASN
1	D	362	ILE
1	D	367	GLN
1	D	418	ASP
1	D	427	ARG
1	E	6	VAL
1	E	11	ARG
1	E	12	ASP
1	E	17	GLN
1	E	49	ARG
1	E	60	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	140	HIS
1	E	148	ASN
1	E	157	LYS
1	E	173	PHE
1	E	183	TYR
1	E	187	GLN
1	E	188	GLU
1	E	199	HIS
1	E	215	GLU
1	E	226	LYS
1	E	229	PHE
1	E	256	SER
1	E	315	VAL
1	E	325	ILE
1	E	327	PHE
1	E	336	TYR
1	E	343	LEU
1	E	346	ASN
1	E	354	ASN
1	E	355	ASN
1	E	363	ARG
1	E	377	LYS
1	E	385	PHE
1	E	428	PHE
1	F	5	ASP
1	F	11	ARG
1	F	28	ILE
1	F	47	MET
1	F	50	TYR
1	F	57	LYS
1	F	64	LYS
1	F	68	GLU
1	F	69	VAL
1	F	102	PHE
1	F	127	VAL
1	F	133	ARG
1	F	135	LEU
1	F	148	ASN
1	F	161	GLU
1	F	162	LYS
1	F	181	ASP
1	F	199	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	207	LYS
1	F	209	PHE
1	F	227	THR
1	F	307	LYS
1	F	331	GLU
1	F	342	ILE
1	F	343	LEU
1	F	350	TRP
1	F	352	ASP
1	F	380	GLU
1	G	10	ILE
1	G	36	LEU
1	G	39	ARG
1	G	48	HIS
1	G	52	GLU
1	G	66	ILE
1	G	116	VAL
1	G	122	ILE
1	G	128	SER
1	G	149	ILE
1	G	158	ILE
1	G	173	PHE
1	G	179	VAL
1	G	181	ASP
1	G	214	ARG
1	G	221	MET
1	G	223	SER
1	G	226	LYS
1	G	229	PHE
1	G	237	LEU
1	G	254	VAL
1	G	256	SER
1	G	258	HIS
1	G	305	GLU
1	G	306	HIS
1	G	308	ASP
1	G	325	ILE
1	G	367	GLN
1	G	369	CYS
1	G	377	LYS
1	G	398	LYS
1	G	413	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	10	ILE
1	H	26	LYS
1	H	45	ASP
1	H	49	ARG
1	H	50	TYR
1	H	57	LYS
1	H	59	LEU
1	H	60	TYR
1	H	91	THR
1	H	98	LEU
1	H	122	ILE
1	H	173	PHE
1	H	179	VAL
1	H	188	GLU
1	H	215	GLU
1	H	221	MET
1	H	223	SER
1	H	226	LYS
1	H	227	THR
1	H	229	PHE
1	H	244	ASP
1	H	275	GLU
1	H	347	LEU
1	H	352	ASP
1	H	355	ASN
1	H	358	ASN
1	H	362	ILE
1	H	371	ARG
1	H	413	ILE
1	I	3	TYR
1	I	102	PHE
1	I	106	LYS
1	I	122	ILE
1	I	173	PHE
1	I	175	PHE
1	I	209	PHE
1	I	221	MET
1	I	228	PHE
1	I	229	PHE
1	I	255	VAL
1	I	258	HIS
1	I	263	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	330	SER
1	I	337	GLU
1	I	346	ASN
1	I	353	VAL
1	I	355	ASN
1	I	357	ASP
1	I	392	ASP
1	I	410	TYR
1	I	418	ASP
1	I	426	LEU
1	J	13	VAL
1	J	50	TYR
1	J	69	VAL
1	J	115	SER
1	J	137	VAL
1	J	140	HIS
1	J	159	LEU
1	J	184	GLU
1	J	214	ARG
1	J	229	PHE
1	J	235	VAL
1	J	237	LEU
1	J	255	VAL
1	J	295	LEU
1	J	298	ARG
1	J	307	LYS
1	J	328	SER
1	J	347	LEU
1	J	348	LEU
1	J	354	ASN
1	J	366	THR
1	J	367	GLN
1	J	371	ARG
1	J	411	SER
1	J	427	ARG
1	K	6	VAL
1	K	26	LYS
1	K	33	ILE
1	K	39	ARG
1	K	52	GLU
1	K	72	LEU
1	K	106	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	116	VAL
1	K	140	HIS
1	K	161	GLU
1	K	173	PHE
1	K	175	PHE
1	K	192	LYS
1	K	199	HIS
1	K	221	MET
1	K	226	LYS
1	K	232	GLN
1	K	274	LEU
1	K	306	HIS
1	K	343	LEU
1	K	352	ASP
1	K	354	ASN
1	K	357	ASP
1	K	364	LEU
1	K	379	MET
1	K	393	LYS
1	K	400	ARG
1	K	402	ASP
1	K	410	TYR
1	L	9	PHE
1	L	12	ASP
1	L	26	LYS
1	L	28	ILE
1	L	52	GLU
1	L	54	LEU
1	L	57	LYS
1	L	58	ARG
1	L	61	GLN
1	L	63	CYS
1	L	76	LEU
1	L	104	GLU
1	L	118	ASP
1	L	165	LEU
1	L	173	PHE
1	L	181	ASP
1	L	189	VAL
1	L	192	LYS
1	L	193	ILE
1	L	199	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	214	ARG
1	L	221	MET
1	L	225	HIS
1	L	228	PHE
1	L	229	PHE
1	L	232	GLN
1	L	291	LEU
1	L	300	PHE
1	L	305	GLU
1	L	325	ILE
1	L	331	GLU
1	L	345	LYS
1	L	346	ASN
1	L	347	LEU
1	L	350	TRP
1	L	362	ILE
1	L	375	LYS
1	L	378	GLU
1	L	404	LYS
1	L	419	GLU
1	L	428	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	199	HIS
1	B	87	ASN
1	B	89	GLN
1	C	199	HIS
1	C	232	GLN
1	D	17	GLN
1	D	140	HIS
1	D	367	GLN
1	E	48	HIS
1	E	344	ASN
1	G	32	ASN
1	G	210	GLN
1	G	225	HIS
1	G	258	HIS
1	G	367	GLN
1	H	199	HIS
1	H	259	HIS

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Mol	Chain	Res	Type
1	I	177	HIS
1	J	140	HIS
1	J	257	ASN
1	J	340	ASN
1	K	262	HIS
1	L	225	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PLP	A	1430	1	15,15,16	1.05	2 (13%)	20,22,23	1.46	3 (15%)
2	PLP	H	1430	1	15,15,16	0.99	1 (6%)	20,22,23	1.46	2 (10%)
2	PLP	J	1430	1	15,15,16	1.02	2 (13%)	20,22,23	1.57	2 (10%)
2	PLP	L	1430	1	15,15,16	1.01	1 (6%)	20,22,23	1.64	2 (10%)
2	PLP	I	1430	1	15,15,16	1.03	1 (6%)	20,22,23	1.66	2 (10%)
2	PLP	K	1430	1	15,15,16	1.03	2 (13%)	20,22,23	1.51	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	B	1430	1	15,15,16	1.04	1 (6%)	20,22,23	1.62	2 (10%)
2	PLP	G	1430	1	15,15,16	1.03	1 (6%)	20,22,23	1.59	2 (10%)
2	PLP	D	1430	1	15,15,16	1.12	1 (6%)	20,22,23	1.73	3 (15%)
2	PLP	E	1430	1	15,15,16	1.17	2 (13%)	20,22,23	2.28	4 (20%)
2	PLP	F	1430	1	15,15,16	1.00	1 (6%)	20,22,23	1.68	2 (10%)
2	PLP	C	1430	1	15,15,16	1.01	1 (6%)	20,22,23	1.81	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	H	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	J	1430	1	-	2/6/6/8	0/1/1/1
2	PLP	L	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	I	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	K	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	B	1430	1	-	3/6/6/8	0/1/1/1
2	PLP	G	1430	1	-	2/6/6/8	0/1/1/1
2	PLP	D	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	E	1430	1	-	2/6/6/8	0/1/1/1
2	PLP	F	1430	1	-	1/6/6/8	0/1/1/1
2	PLP	C	1430	1	-	4/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1430	PLP	C3-C2	-3.21	1.37	1.40
2	E	1430	PLP	C3-C2	-3.12	1.37	1.40
2	K	1430	PLP	C3-C2	-2.69	1.38	1.40
2	B	1430	PLP	C3-C2	-2.63	1.38	1.40
2	G	1430	PLP	C3-C2	-2.62	1.38	1.40
2	A	1430	PLP	C3-C2	-2.62	1.38	1.40
2	J	1430	PLP	C3-C2	-2.62	1.38	1.40
2	I	1430	PLP	C3-C2	-2.58	1.38	1.40
2	F	1430	PLP	C3-C2	-2.40	1.38	1.40
2	L	1430	PLP	C3-C2	-2.37	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1430	PLP	C3-C2	-2.35	1.38	1.40
2	H	1430	PLP	C3-C2	-2.30	1.38	1.40
2	A	1430	PLP	O4P-C5A	-2.15	1.37	1.45
2	J	1430	PLP	O4P-C5A	-2.02	1.37	1.45
2	K	1430	PLP	O4P-C5A	-2.01	1.37	1.45
2	E	1430	PLP	O4P-C5A	-2.00	1.37	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1430	PLP	O4P-C5A-C5	6.87	122.44	109.35
2	C	1430	PLP	O4P-C5A-C5	6.47	121.68	109.35
2	F	1430	PLP	O4P-C5A-C5	5.92	120.64	109.35
2	E	1430	PLP	C4A-C4-C5	5.72	126.83	120.94
2	D	1430	PLP	O4P-C5A-C5	5.58	119.98	109.35
2	I	1430	PLP	O4P-C5A-C5	5.36	119.57	109.35
2	J	1430	PLP	O4P-C5A-C5	5.35	119.55	109.35
2	L	1430	PLP	O4P-C5A-C5	5.17	119.20	109.35
2	B	1430	PLP	O4P-C5A-C5	5.12	119.10	109.35
2	H	1430	PLP	O4P-C5A-C5	4.79	118.48	109.35
2	K	1430	PLP	O4P-C5A-C5	4.78	118.47	109.35
2	G	1430	PLP	O4P-C5A-C5	4.76	118.43	109.35
2	A	1430	PLP	O4P-C5A-C5	4.48	117.90	109.35
2	L	1430	PLP	C4A-C4-C5	3.38	124.41	120.94
2	D	1430	PLP	C4A-C4-C5	3.25	124.28	120.94
2	I	1430	PLP	C4A-C4-C5	3.22	124.25	120.94
2	G	1430	PLP	C4A-C4-C5	3.09	124.12	120.94
2	K	1430	PLP	C4A-C4-C5	2.95	123.98	120.94
2	B	1430	PLP	C4A-C4-C5	2.95	123.97	120.94
2	E	1430	PLP	C4A-C4-C3	-2.91	115.56	120.50
2	C	1430	PLP	C4A-C4-C5	2.85	123.87	120.94
2	F	1430	PLP	C4A-C4-C5	2.73	123.74	120.94
2	H	1430	PLP	C4A-C4-C5	2.43	123.44	120.94
2	A	1430	PLP	C5-C6-N1	-2.18	120.19	123.82
2	A	1430	PLP	C6-C5-C4	2.15	119.85	118.16
2	E	1430	PLP	C5A-C5-C6	-2.09	115.93	119.37
2	J	1430	PLP	C5-C6-N1	-2.04	120.42	123.82
2	D	1430	PLP	C2A-C2-C3	-2.02	118.39	120.89

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1430	PLP	C5A-O4P-P-O2P
2	B	1430	PLP	C5A-O4P-P-O3P
2	C	1430	PLP	C4-C5-C5A-O4P
2	C	1430	PLP	C6-C5-C5A-O4P
2	C	1430	PLP	C5A-O4P-P-O2P
2	C	1430	PLP	C5A-O4P-P-O3P
2	E	1430	PLP	C4-C5-C5A-O4P
2	E	1430	PLP	C6-C5-C5A-O4P
2	G	1430	PLP	C5A-O4P-P-O2P
2	G	1430	PLP	C5A-O4P-P-O3P
2	H	1430	PLP	C5A-O4P-P-O2P
2	H	1430	PLP	C5A-O4P-P-O3P
2	I	1430	PLP	C5A-O4P-P-O2P
2	I	1430	PLP	C5A-O4P-P-O3P
2	J	1430	PLP	C5A-O4P-P-O1P
2	K	1430	PLP	C5A-O4P-P-O1P
2	K	1430	PLP	C5A-O4P-P-O2P
2	K	1430	PLP	C5A-O4P-P-O3P
2	L	1430	PLP	C5A-O4P-P-O2P
2	B	1430	PLP	C5A-O4P-P-O1P
2	H	1430	PLP	C5A-O4P-P-O1P
2	I	1430	PLP	C5A-O4P-P-O1P
2	L	1430	PLP	C5A-O4P-P-O3P
2	L	1430	PLP	C5A-O4P-P-O1P
2	F	1430	PLP	C5A-O4P-P-O2P
2	J	1430	PLP	C5A-O4P-P-O2P

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1430	PLP	2	0
2	J	1430	PLP	1	0
2	B	1430	PLP	1	0
2	G	1430	PLP	1	0
2	E	1430	PLP	2	0
2	F	1430	PLP	2	0
2	C	1430	PLP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	426/429 (99%)	-0.80	0 100 100	30, 45, 66, 73	0
1	B	424/429 (98%)	-0.79	0 100 100	31, 47, 68, 80	0
1	C	420/429 (97%)	-0.77	0 100 100	34, 52, 67, 79	0
1	D	425/429 (99%)	-0.65	0 100 100	33, 61, 78, 85	0
1	E	427/429 (99%)	-0.63	1 (0%) 95 87	40, 62, 80, 95	0
1	F	418/429 (97%)	-0.64	0 100 100	43, 62, 76, 93	0
1	G	429/429 (100%)	-0.84	0 100 100	30, 45, 61, 71	0
1	H	427/429 (99%)	-0.78	0 100 100	29, 47, 71, 79	0
1	I	427/429 (99%)	-0.82	0 100 100	33, 48, 64, 71	0
1	J	429/429 (100%)	-0.71	0 100 100	37, 53, 72, 78	0
1	K	422/429 (98%)	-0.62	0 100 100	45, 62, 76, 91	0
1	L	420/429 (97%)	-0.54	0 100 100	51, 66, 79, 93	0
All	All	5094/5148 (98%)	-0.72	1 (0%) 100 100	29, 55, 74, 95	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	355	ASN	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	L	1430	15/16	0.92	0.21	65,66,66,66	0
2	PLP	I	1430	15/16	0.93	0.21	41,42,42,43	0
2	PLP	C	1430	15/16	0.94	0.20	45,46,46,47	0
2	PLP	K	1430	15/16	0.94	0.18	58,59,59,60	0
2	PLP	D	1430	15/16	0.94	0.19	53,56,59,60	0
2	PLP	J	1430	15/16	0.95	0.13	47,47,47,48	0
2	PLP	A	1430	15/16	0.96	0.15	36,37,39,39	0
2	PLP	B	1430	15/16	0.97	0.14	41,43,44,44	0
2	PLP	E	1430	15/16	0.97	0.17	43,44,46,47	0
2	PLP	F	1430	15/16	0.97	0.20	51,54,56,57	0
2	PLP	G	1430	15/16	0.97	0.18	37,37,39,39	0
2	PLP	H	1430	15/16	0.98	0.14	42,44,45,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.